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Techno-economic assessment and uncertainty analysis of thermochemical processes for second generation biofuels

Ioanna Dimitriou

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Aston University

TECHNO-ECONOMIC ASSESSMENT AND UNCERTAINTY ANALYSIS OF THERMOCHEMICAL PROCESSES FOR SECOND GENERATION TRANSPORT BIOFUELS

IOANNA DIMITRIOU

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Thesis Summary

Biomass-To-Liquid (BTL) is one of the most promising low carbon processes available to support the expanding transportation sector. This multi-step process produces hydrocarbon fuels from biomass, the so-called “second generation biofuels” that, unlike first generation biofuels, have the ability to make use of a wider range of biomass feedstock than just plant oils and sugar/starch components. A BTL process based on gasification has yet to be commercialized. This work focuses on the techno-economic feasibility of nine BTL plants. The scope was limited to hydrocarbon products as these can be readily incorporated and integrated into conventional markets and supply chains.

The evaluated BTL systems were based on pressurised oxygen gasification of wood biomass or bio-oil and they were characterised by different fuel synthesis processes including: Fischer-Tropsch synthesis, the Methanol to Gasoline (MTG) process and the Topsoe Integrated Gasoline (TIGAS) synthesis. This was the first time that these three fuel synthesis technologies were compared in a single, consistent evaluation. The selected process concepts were modelled using the process simulation software IPSEpro to determine mass balances, energy balances and product distributions. For each BTL concept, a cost model was developed in MS Excel to estimate capital, operating and production costs. An uncertainty analysis based on the Monte Carlo statistical method, was also carried out to examine how the uncertainty in the input parameters of the cost model could affect the output (i.e. production cost) of the model. This was the first time that an uncertainty analysis was included in a published techno-economic assessment study of BTL systems.

It was found that bio-oil gasification cannot currently compete with solid biomass gasification due to the lower efficiencies and higher costs associated with the additional thermal conversion step of fast pyrolysis. Fischer-Tropsch synthesis was the most promising fuel synthesis technology for commercial production of liquid hydrocarbon fuels since it achieved higher efficiencies and lower costs than TIGAS and MTG. None of the BTL systems were competitive with conventional fossil fuel plants. However, if government tax take was reduced by approximately 33% or a subsidy of £55/t dry biomass was available, transport biofuels could be competitive with conventional fuels. Large scale biofuel production may be possible in the long term through subsidies, fuels price rises and legislation.

Keywords: biomass, gasification, pyrolysis, synthetic fuels, process simulation

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Abbreviations

ACR	Annual Capital Repayment
ASU	Air Seperation Unit
bbl	Oil barrel
BCL	Battelle Columbus Laboratory
BG	Biomass Gasification
BIG-FT	Biomass Integrated Gasification-Fischer Tropsch
BTL	Biomass-To-Liquids
CCS	Carbon Capture and Storage
CFB	Circulating Fluidised Bed
COD	Conversion of low molecular weight Olefins to Diesel
CPI	Consumer Price Index
CPO_x	Catalytic Partial Oxidation
CTL	Coal-To-Liquids
DEA	Diethanolamine
DECC	Department of Energy and Climate Change
DME	Dimethyl Ether
daf	dry ash-free
ECN	Energy Research Institute of the Netherlands
EF	Entrained Flow
EU	European Union
FT	Fischer-Tropsch
GTI	Gas Technology Institute
GTL	Gas-To-Liquids
HGT	Heavy Gasoline Treatment
HHV	Higher Heating Value
HPC	Heavy Paraffin Conversion
HPS	Heavy Paraffin Synthesis
HT	High Temperature
HTFT	High Temperature Fischer-Tropsch
HTW	High Temperature Winkler
KIT	Karlsruhe Institute of Technology
LO-CAT	Liquid Oxidation Catalyst
LT	Low Temperature
LTFT	Low Temperature Fischer-Tropsch
LHV	Lower Heating Value

MC	Monte Carlo
MDEA	Methyldiethanolamine
MDK	Model Development Kit
MDL	Model Development Language
MeOH	Methanol
MOGD	Methanol to Olefins Gasoline and Diesel
MTG	Methanol to Gasoline
MTO	Methanol To Olefins
MTP	Methanol To Propylene
NREL	National Renewable Energy Laboratory
O&M	Operating & Maintenance
PGP_Lib	Pyrolysis and Gasification Process Library
ppmV	parts per million volume
ppmw	parts per million weight
PNL/PNNL	Pacific Northwest National Laboratory
PSE	Process Simulation Environment
RO	Renewables Obligation
RSH	Reception, Storage and Handling
RTFO	Renewable Transport Fuel Obligation
RTFC	Renewable Transport Fuel Certificate
SMDS	Shell Middle Distillate Synthesis
SMR	Steam Methane Reformer
SNG	Substitute Natural Gas
SRC	Short Rotation Coppice
SSD	Superheated Steam Dryer
SSPD	Sasol Slurry Phase Distillate
TCI	Total Capital Investment
TOPs	Torrefied Pellets
TPC	Total Plant Cost
TPEC	Total Purchased Equipment Cost
UKPIA	UK petroleum industry association
UN	United Nations
waf	water ash-free
WGS	Water-Gas-Shift
WPIF	Wood Panel Industries Federation

Symbols

C_p	heat capacity	J/mol·K
H_i	enthalpy of model substance	kJ/kg
$\dot{h}$	enthalpy flow	kJ/h
h^*	IPSEpro stream enthalpy	kJ/kg
Q_{clg}	cooling duty	kW
Q_{htx}	heating duty	kW
Q_{loss}	heat loss	kW
M	molecular weight	g/mol
$\dot{m}$	massflow	kg/h
N	plant life	years
r	interest rate	%
T	temperature	^{o}C, K
w	weight fraction	kg/kg
y	yield	%
$\Delta h^0_{f,298}$	enthalpy of formation	kJ/mol
η	energy efficiency	%
λ	stoichiometric air-fuel ratio	kg/kg

1 INTRODUCTION

1.1 Background

Energy is a critical resource that governs the lives of humanity and promotes civilization. Energy services around the world have provided comfort through transportation, power and heat, however there is a considerable and widespread concern over the effect of the extensive consumption of energy on the environment and security for those countries with limited energy resources.

Over the last decades, significant amounts of carbon dioxide (CO_2), which is a greenhouse gas, have been accumulated in the atmosphere. Since the Industrial Revolution, humans have significantly added to the amount of heat-trapping greenhouse gases in the atmosphere by burning fossil fuels, cutting down forests and other activities. It is believed that the recent increase in man-made greenhouse gas (GHG) emissions is the main reason behind the observed rise in average global temperatures [1]. As pressure to reduce GHG grows, several countries have ratified the Kyoto Protocol (1997), which is an agreement made under the UN Framework Convention on Climate Change for the reduction of GHG [2]. The major feature of the Kyoto Protocol is that the industrialised countries that ratify this protocol commit to mandatory GHG emissions reductions. Specifically for the Member States of the European Union (EU), this corresponds to a reduction of 5% below 1990 levels by 2008 - 2012 [2].

In addition to environmental concerns and according to the current facts, energy experts predict a 35% increase in worldwide petroleum demand by 2025 [3]. This will increase dependency on a limited number of oil producing countries with grave risks for energy security and global social stability [4]. Regarding the oil market, it is predicted that the Middle East will continue to be in dominant position as it has the greatest proven oil reserves in the world. Conversely, nations with less petroleum resources will be vulnerable to energy shortages unless they develop alternative sources of energy. Such alternatives include nuclear, wind, solar, hydroelectricity, wave, tidal, geothermal and bioenergy.

Biomass derived transportation fuels (biofuels) can play an important role in filling the gap between limited fuel supplies and increasing worldwide demand. Biomass is the only

carbon neutral alternative source for the production of liquid fuels thus it can constitute a key option to deliver significant reductions in GHG emissions from the transportation sector. Contrary to electricity or heat production, where the relevant technologies can be operated in a carbon neutral way by using CO_2 sequestration, the transportation sector does not allow CO_2 capture due to the nature of transport emissions. Therefore, the substitution of fossil fuels by biofuels constitutes the only way to reduce GHG emissions from transport [5]. This is also why the European Union has set ambitious targets for the application of biofuels through EU Biofuels Directive 2009/28/EC. According to the directive, 10% of all transport fossil fuels sold in EU countries, calculated on the basis of energy content, should be replaced with biofuels by 2020 [6]. The UK's implementation of the EU Biofuels Directive is the Renewable Transport Fuel Obligation (RTFO). The main requirement of the RTFO is that biofuels should contribute over 5%, by volume, of road vehicle fuels sold in the UK by April 2013 [7].

Nowadays, the substitution of transport fossil fuels with biofuels is already feasible by state-of-the-art renewable liquid hydrocarbons, such as bioethanol for gasoline engines, produced by fermentation of sugar or starch and biodiesel for diesel engines produced via transesterification of vegetable oils or animal fats [8]. These so-called "first generation biofuels" are characterised by an unexpected growth following government subsidies and legislative pressures, however there are some serious problems associated with their application with respect to feedstock requirements and land availability. In the UK, the road transport sector consumes 37.8 million tonnes of crude oil products per year [8]. In order to meet current usage, 12.3 million ha and 7.8 million ha of land would be required for rape cultivation and sugar beet production [8]. Since the total area of arable land in the UK is 6.5 million ha [8], first generation biofuels do not constitute a feasible solution for meeting the current UK transport requirements. In addition to the consequences on economy and land competition, net carbon savings from first generation biofuels are questionable due to the clearance of virgin land (e.g. rain forests) for cultivation, high fertilizer requirement and low productivity per hectare [4].

In order to overcome the above mentioned shortages, the so-called "second generation biofuels" have been introduced. Unlike first generation biofuels, they have the ability to make use of a wider range of biomass feedstocks than just plant oils and sugar/starch components. These sources include non-food biomass, dedicated energy crops and

biomass co-products and waste from many different sectors such as agriculture, horticulture, forestry and paper and pulp processing [9]. The processing of these ligno-cellulosic biomass feedstocks by thermal conversion is considered to be a long-term prospect for renewable transport fuels production [10].

Second generation hydrocarbon biofuels are specifically attractive due to their unlimited compatibility with conventional fuels in any proportion and the capability to be refined to current fuel standards and specifications in conventional refineries, thus offering economies of scale and access to state-of-the-art processing. Development of thermal processing technologies for the production of second generation biofuels is already well advanced in some areas, especially gasification, which presents higher thermal efficiencies compared to combustion, whereas fast pyrolysis is still at an early stage of development [11].

1.2 Scope and objectives of the thesis

This study was funded by the Engineering and Physical Sciences Research Council (EPSRC) as part of the SUPERGEN Bioenergy II Consortium which was concerned with the development of energy from biomass. This consortium consisted of leading academic and industrial partner organisations across the UK who organised the work into eight integrated and coordinated themes that are listed below and shown in Figure 1-1.

1. Resources (Subtheme: Marine Biomass)
2. Characterisation and Pre-treatment (Subtheme: Nitrogen)
3. Thermal Conversion
4. Power and Heat
5. Transport Fuels, Biorefinery (Subtheme: Ammonia)
6. Systems Analysis
7. Innovation
8. Dissemination

The present study was carried out as part of Theme 5 of this programme and focused on transport fuels. Aston University was the leader of Theme 5 and had responsibility for a number of tasks within this theme including the production of hydrocarbon fuels and chemicals from biomass derived syngas via Fischer-Tropsch synthesis.

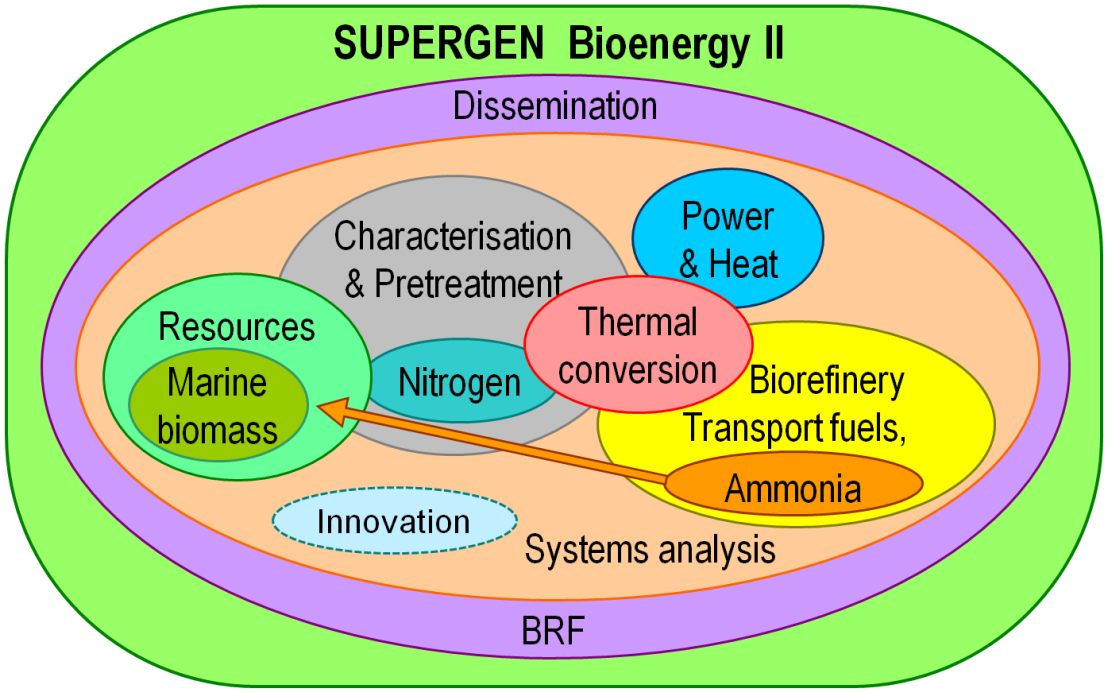

Figure 1-1: The structure of SUPERGEN Bioenergy II

This work examines processes from solid biomass to liquid transport fuels, known as Biomass-To-Liquids (BTL) processes. The term "BTL" is only applied to thermo-chemical processes, such as pyrolysis and gasification, and thus it is not used for biochemical routes (e.g. fermentation) to biofuel production. The scope was limited to hydrocarbon products (diesel, gasoline and kerosene) as these can be readily incorporated and integrated with conventional markets and supply chains while alcohols (e.g. ethanol, methanol, mixed alcohols) and ethers (e.g. DME – dimethyl ether) have more limited short term prospects in the UK and European transport fuel infrastructures [12].

The main objectives of this thesis are as follows:

- Identify the most promising thermo-chemical process routes in terms of performance and costs for large-scale production of 2nd generation liquid transport biofuels, including options for biomass pre-treatment (e.g. fast pyrolysis), gasification technologies, syngas clean-up and fuel synthesis processes.
- Measure the technical performance in terms of energy efficiency and mass yield of the selected process concepts by using the process simulation software IPSEpro to determine mass balances, energy balances and product distributions.

- Develop an economic model for each process concept to estimate capital, operating and production costs.
- Compare the selected process concepts in terms of performance and costs.
- Conduct a sensitivity analysis on production costs with respect to key performance and economic parameters.
- Carry out an uncertainty analysis to examine how the uncertainty in the economic model parameters can affect production costs.
- Estimate the minimum subsidy required for biofuels to compete with conventional transport fuels.

1.3 Thesis structure

Chapter 2 describes the basic features and status of the various technology options available for the production of liquid hydrocarbon fuels in order to identify the most suitable technologies for commercial biofuel production.

Chapter 3 reviews previous techno-economic studies of BTL systems. The scope, results, strengths and weaknesses of a number of recent comparative studies are highlighted to develop a scope for this work that supplements previous studies and builds on experience already gained.

Chapter 4 discusses the selection of the BTL plant concepts identified as most promising for techno-economic evaluation, whereas Chapter 5 describes the development of the process simulation models that are used to evaluate the selected BTL concepts. The chapter concludes with a performance comparison in terms of energy efficiency and mass yield of the selected systems.

Chapter 6 discusses the methodology which was used to economically evaluate the selected BTL concepts which are compared in terms of capital, operating and production costs. The chapter also addresses uncertainties in the economic parameters and examines whether BTL plants could compete economically with conventional transport fuels plants.

Chapter 7 summarises the findings of this work and draws conclusions from the systems' evaluations. The thesis ends with recommendations for further work in Chapter 8.

2 TECHNOLOGIES NECESSARY FOR BIOFUEL SYNTHESIS

2.1 Introduction

This chapter provides an overview of various thermo-chemical conversion technologies associated with the production of liquid hydrocarbon fuels. It describes the main technologies of biomass pre-treatment, gasification, gas cleaning and conditioning and fuel synthesis. This overview cannot properly consider all aspects of the available technologies for biofuel production as this is out of the scope of this thesis but identifies the main advantages and disadvantages of these technologies and briefly discusses them. The findings of this overview led to the selection of the most promising technologies for commercial transport biofuel production which is discussed in Chapter 4.

Biomass-to-Liquid (BTL) is a multi-step process that converts biomass to liquid biofuels through thermo-chemical routes. It consists of several discrete steps which are discussed in the next sections [12]:

- Reception storage and handling
- Preparation including comminution, screening, drying
- Pre-treatment as fast pyrolysis or torrefaction (optional)
- Gasification of solid biomass (fresh or torrefied) or bio-oil from fast pyrolysis
- Gas cleaning to derive correct gas quality
- Gas conditioning to derive correct gas composition
- Synthesis of hydrocarbons (or methanol or alcohols)
- Conversion of methanol to gasoline and/or diesel (optional)
- Synthesis products refining
- Offsites including an oxygen production plant (optional) and power and heat provision

2.2 Reception, storage and handling (RSH)

Conversion of biomass into a more valuable product requires that after harvesting, the material is transported to the conversion plant where it is stored and reclaimed for preparation and pre-treatment. A simple concrete pad with a front end loader can be used for biomass storage in small-scale plants, whereas substantial automated bulk handling

systems analogous to those found on pulp and paper mills can be used in large capacity plants [12].

A wide variety of biomass sources can be used as feedstock for the production of 2nd generation liquid fuels. Such sources range from wood (logging residues, trees, wood wastes, SRC), energy crops (miscanthus and switchgrass) and agricultural wastes (e.g. straw) [8, 13]. The elemental composition along with the heating value of the biomass employed is required for the estimation of mass and energy balances. In Table 2-1 such data is given for several types of biomass.

Table 2-1: Composition & calorific values of different types of biomass (wt% dry, ash free) [14]

Biomass	**C**	**H**	**O**	**N**	**S**	**Cl**	**HHV (MJ/kg)**	**LHV (MJ/kg)**
Wood chips	50.8	6.2	42.4	0.5	0.05	0.013	20.7	19.4
Miscanthus	49.1	6.4	43.9	0.3	0.1	0.132	19.9	18.5
Switchgrass	49.2	6	43.9	0.77	0.08	0.036	19.3	18
Wheat straw	48.5	5.8	43.6	1.74	0.11	0.263	19.4	18.1
Rice straw	48.1	5.9	43.6	1.69	0.14	0.581	19.7	18.4

2.3 Preparation

Biomass requires several preparation steps, the number of which is determined by the type of biomass. These steps include:

- Comminution to reduce biomass material size to the necessary size for the subsequent conversion step.
- Screening to separate the required biomass particle size. This may include rejection of oversized particles for recycling to a re-chipper and/or rejection of the undersized particles which can potentially be used elsewhere in the plant (e.g. combustion for heat provision to the drier).
- Drying to reduce biomass moisture content to the preferred level for the subsequent conversion step.
- Optional steps, such as magnetic separation to remove ferrous metals. These steps depend on the type of biomass used in the process.

Biomass feedstocks are typically characterised by relatively high water contents (up to 65%) [8]. For biomass gasification (BG) applications, drying is usually required to reduce the moisture content to 10-15% wt for efficient operation of the gasifier [8, 15, 16]. For fast pyrolysis, the moisture content of the feed material should be reduced to a maximum 10% [17].

2.4 Pre-treatment

In addition to biomass preparation, further thermal pre-treatment may be desirable for certain biomass feedstocks or gasification technologies. Fast pyrolysis and torrefaction have attracted considerable interest as methods of pre-treatment for biomass since both technologies can convert biomass into high energy dense carriers to ease transportation and handling.

2.4.1 Fast pyrolysis

2.4.1.1 Process description

Pyrolysis is the thermal decomposition of the organic components in biomass in the absence of oxygen to produce a mixture of solid char, condensable liquids and gases. The relative proportions of the products depend on the pyrolysis method, the biomass characteristics and the reaction parameters [18, 19]. Fast pyrolysis is a moderate temperature (around 500^{o}C) process that devolatilises biomass into high yields of a liquid known as bio-oil (up to 75 wt%), with some char (typically 13 wt%) and gas (typically 12 wt%).

Bio-oil yields can be maximised with short vapour residence times of typically 1 second, rapid cooling of pyrolysis vapours, high heating rates and moderate temperatures of around 500^{o}C [20]. Typical bio-oils have a high oxygen content up to about 45 wt% and may contain up to 35 % water [17, 21]. The main characteristics of bio-oil are summarised in Table 2-2.

Figure 2-1 shows a typical fast pyrolysis process based on the fluidised bed reactor technology. After preparation, which usually includes drying and grinding, the biomass is fed into the reactor via a conveyor screw.

Table 2-2: Typical characteristics of wood-derived bio-oil [17, 22]

Moisture content pH Specific gravity	25% 2.5 1.20
Elemental analysis (moisture free basis) C H O N	 56% 6% 38% 0-0.1%
Higher heating value, HHV as produced (depends on moisture)	17.0 MJ/kg
Viscosity (at 40^{o}C and 25% water)	40-100 cP

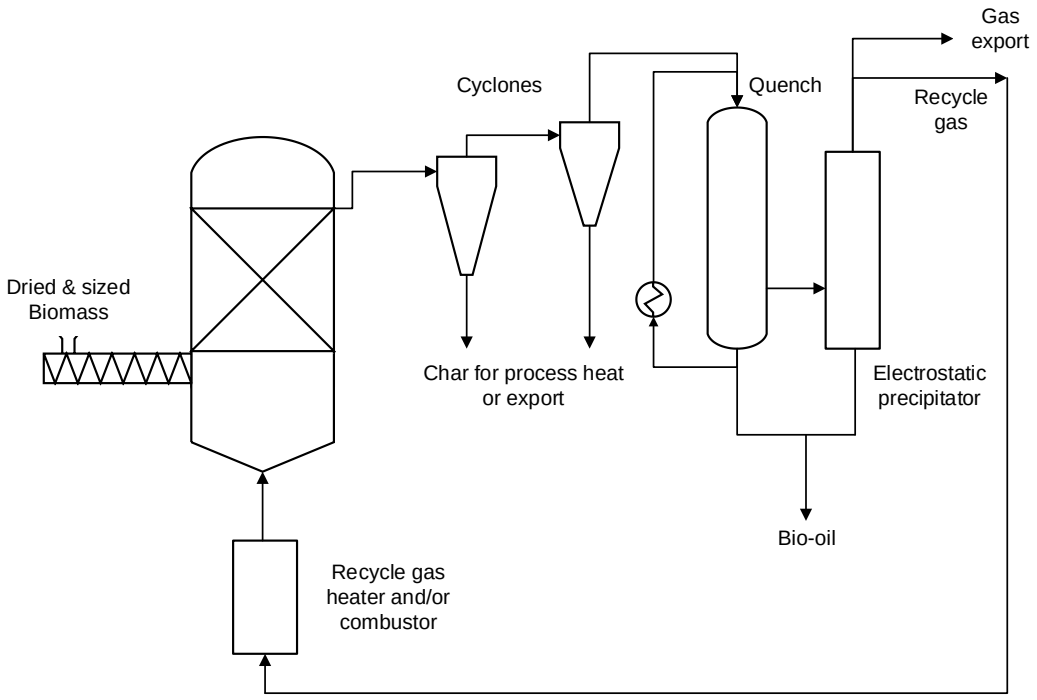

Figure 2-1: Typical fast pyrolysis process

The heat for both pyrolysis and drying may be provided by the combustion of parts or all of the non-condensable gases and char, depending on temperature. The char is separated in a set of cyclones, after which the vapours are condensed to give the bio-oil. Electrostatic precipitation has been shown to be the most effective method for collection of aerosols which are formed during the condensation of pyrolysis vapours [17]. Extensive reviews of biomass fast pyrolysis are available [11, 17, 22, 23].

2.4.1.2 Bio-oil gasification for synfuels

As discussed below, there is an increasing interest in using bio-oil and bio-oil/char slurries as energy carriers to feed state-of-the-art gasifiers for liquid fuels synthesis plants. Even though the additional thermal step of fast pyrolysis reduces overall process efficiency [5, 17], there are some important advantages associated with this option:

- **Easier and cheaper transportation**

  Biomass has a much lower bulk density (100-150 kg/m^3) compared to bio-oil (1200 kg/m^3), thus due to the lower volume of feed material this option results in lower transportation costs [12, 17]. In addition, the energy content of bio-oil is about the same as biomass which, in combination with bio-oil's higher bulk density, leads to higher energy densities than biomass [5, 12, 17].

- **Need for pre-treatment for certain gasifiers**

  Fast pyrolysis, along with other upgrading technologies, is considered crucial for entrained flow gasifiers since this technology requires very fine particles by milling of solid biomass which is very energy consuming [17, 24].

- **Lower gas cleaning requirements**

  Biomass contains alkali metals (see section 2.6.3) which can cause significant problems as they can damage filters at high temperature and poison synthesis catalysts [25]. In fast pyrolysis these compounds are almost entirely retained in the char which, as explained earlier, is typically separated from bio-oil in a series of cyclones. Therefore, the product gas from the gasifier fed with bio-oil will have much lower alkali metals thus reducing cleaning requirements [12].

- **Combining decentralisation and economies of scale**

  An interesting concept is to have a number of smaller fast pyrolysis plants that produce bio-oil which is then shipped to a large scale decentralised gasification and fuel synthesis plant for further conversion to transport fuels. Although this concept will result in lower process efficiencies and higher transportation costs, these are believed to be more than compensated by the economies of scale achievable on a commercial sized gasification/synthesis plant [5, 17]. This concept is being investigated by FZK in collaboration with Lurgi (Bioliq project) although, in this case, bio-oil is mixed with the pyrolysis char to create a slurry for subsequent

gasification to syngas and conversion to fuels and/or chemicals (see section 2.11.4). Consequently, the energy needs of the fast pyrolysis process need to be met by another source.

2.4.2 Torrefaction

Torrefaction is thermal treatment technology performed at atmospheric pressure at 200-300^{o}C in the absence of oxygen [26]. Torrefaction dries and partially devolatilises biomass through decomposition of some of the hemicellulose to give a dry and fragile form of biomass that can be crushed and milled [12]. The solid biomass product has a very low moisture content (1% to 6%) and a high calorific value compared to fresh biomass [19]. A flow diagram of the torrefaction process is shown in Figure 2-2. Torrefaction is considered to be a promising option for feeding biomass into entrained flow gasifiers which are likely to be preferred for large-scale biofuel production [26]. The suitability of entrained flow gasifiers for large scale BTL plants is discussed in detail in section 4.5.

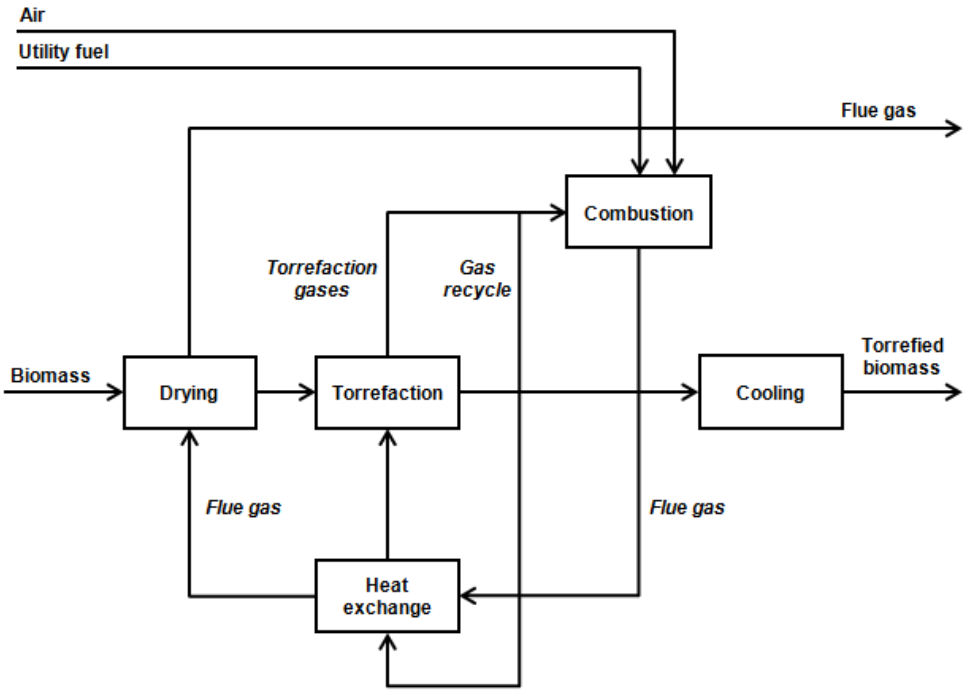

Figure 2-2: The ECN torrefaction process

Torrefaction requires additional heat above 300^{o}C in order to drive the drying and devolatilisation process. In the case of fast pyrolysis, the char and the non condensable gases can be used to supply the necessary heat for the reactions of fast pyrolysis.

However, as shown in Figure 2-2 above, torrefaction only has the off-gas for heat supply. This will contain some particulates which will require satisfactory removal [12]. ECN, who are the main proponents of torrefaction, report that the mass and energy yield of the process is 70% and 90%, respectively [27]. They also claim that the heating requirements of the process can be fulfilled by combusting the off-gas [27, 28] but there is no evidence or experience of this claim. At the high yields claimed it is questionable whether there is sufficient energy in the off-gas to cover the heat requirements of the process and also whether the off-gas quality is sufficiently high to sustain combustion [12]. Therefore it is likely that other energy sources for heat supply will be required such as fresh biomass or torrefied product [12]. Unlike fast pyrolysis, torrefaction is not commercialised yet and has only been demonstrated under laboratory conditions [19].

2.5 Gasification

Gasification is a high temperature process that converts a carbonaceous feedstock, such as coal or biomass, into gas. This gas product, known as syngas (from synthetic gas or synthesis gas) or producer gas, contains carbon monoxide, hydrogen, carbon dioxide, methane, water, nitrogen (if air is used as the oxidation medium) and various contaminants such as small char particles, tars and ash. Gasification occurs in three main steps: - pre-heating and drying to evaporate moisture, - pyrolysis to produce gas, volatiles and char, - syngas formation through gasification or partial oxidation of the char residues, pyrolysis vapours and pyrolysis gases [11, 23].

2.5.1 Gasification agent

Air, oxygen, steam or a mixture of these can be used as gasification medium. Partial oxidation with air produces a low heating value gas around 5 MJ/m^3, which is heavily diluted with nitrogen [11, 29]. This is disadvantageous for the subsequent synthesis since nitrogen dilutes carbon monoxide and hydrogen in synthesis gas thus it adversely affects the synthesis reaction resulting in poor performance. Moreover, due to the high volume of nitrogen larger downstream equipment is required which results in increased capital costs [23].

Oxygen gasification gives a better quality (heating value: 10-12 MJ/m^3), nitrogen-free syngas [11, 30]. However, oxygen plants require additional capital costs and energy requirements due to the need for air separation.

The heating value of syngas is maximised during steam gasification (or indirect gasification) of biomass (~15-20 MJ/m^3) due to a higher CH_4 and hydrocarbon gas content [11]. However, the higher methane content gas increases the process complexity and costs if the preferred product is liquid biofuels as the lower hydrocarbons need to be reformed to syngas. Nevertheless, for SNG production, this route has advantages [12].

2.5.2 Pressure

Gasification can take place both in atmospheric and elevated pressures. Pressurised operation has the advantage of avoiding a costly compression step before the synthesis process however it is related to problems with regard to biomass feeding into the pressurised gasification system (see section 2.4.1.2). The feasibility of biomass gasification has already been demonstrated both at atmospheric pressure as well as in pressurized systems. More specifically:

At atmospheric pressure, the ARBRE demonstration plant was installed from 1998 to 2001 in Eggborough, Yorkshire, UK. The BIGCC-plant (biomass integrated gasification combined cycle) was designed for a biomass fuel power of approximately 23 MW and used a catalytic cracker for tar cleaning. After further cleaning and a 5-stage compression, the synthesis gas passed through a gas turbine, with heat recovery in a steam cycle. In total, a net electricity production of 8 MW was anticipated, although the plant only operated for 48 hours in total, corresponding to an anticipated electric efficiency of about 30% [31-33].

Biomass atmospheric gasification has been demonstrated successfully in a 8MW_{th} CHP plant in Guessing, Austria. After steam gasification, gas cleaning and cooling, the syngas is combusted in a gas engine with a subsequent steam cycle. The plant has been operational since 2002 [34]. The unit has achieved more than 70,000 hours of operation at a plant availability in excess of 90% [33].

A pressurized CFB air gasifier was demonstrated in the Värnamo plant in Sweden. After gasification at 18 bar, only hot gas cleaning was required before combustion in a gas turbine with a subsequent steam cycle. A net electric output of 6 MW was achieved, with an additional 9 MW of district heat production [32, 35].

2.5.3 Reactors

A number of biomass gasification reactors have been developed and tested as shown in Table 2-3. Each main type of gasifier is summarised below with significant advantages and limitations highlighted.

Table 2-3: Gasifier technologies [11, 23]

Gasifier type	**Characteristics**
Downdraft-fixed bed reactor	• Solid and product gas move downward in a co-current mode • A relatively clean gas is produced with low tar • Limited scale-up potential to about 500kg/h feed rate • Reliable and proven technology for feedstocks with low content of fine particles
Updraft-fixed bed reactor	• Solid moves down and product gas moves upward in a counter-current mode • Low quality gas is produced with high tar content • Small scale-up potential (around 4 t/h feed rate) • Reliable and proven technology for feedstocks with low content of fine particles • Simple construction and high thermal efficiency
Bubbling Fluidised bed (BFB)	• Air or oxygen blown up though the fluidising medium (e.g. silica sand) bed to mix with biomass. • High reaction rates & isothermal bed operation • Moderate tar content in product gas but higher particulates • Suitable for large scale applications since they can be readily scaled up to about 10-15 dry t/h with high specific capacity • Small carbon loss with ash
Circulating Fluidised bed (CFB)	• All features of the BFB plus • Higher carbon conversion efficiency since entrained solid material is recycled back to the fluid bed • Only potentially viable above 15 dry t/h feed rate
Entrained flow	• Costly feedstock pre-treatment is needed since very small particles can be processed. • Product gas has low concentrations of tars and condensable gases • Operate at higher temperatures of about 1200 – 1500 ^{o}C • Large minimum size for viability, above around 20 dry t/h feed rate

This study cannot properly consider all aspects of biomass gasification as this is out of the scope of the thesis. Extensive reviews of biomass gasification are available [11, 23, 25, 36, 37].

2.6 Gas cleaning

The syngas produced by the gasification process contains several impurities (tars, particulates, alkali compounds, H_2S, HCl, NH_3 and HCN) that need to be removed prior to fuel synthesis mainly due to the high sensitivity of synthesis catalysts to small amounts of these contaminants. Table 2-4 summarises the main problems associated with these impurities and common clean-up methods.

Table 2-4: Syngas contaminants [30]

Contaminant	**Problems**	**Clean-up method**
Particulates (ash, char, bed material fines)	Erosion	Filtration, scrubbing
Alkali metals (sodium & potassium compounds)	Hot corrosion	Cooling, adsorption, condensation, filtration
Nitrogen and chlorine compounds (NH_3, HCl)	Corrosion & NO_x formation respectively	Scrubbing, dolomite absorption in tar cracker (if used)
Tars (mostly poly-nuclear aromatics)	Clogged filters, deposit internally	Tar catalytic cracking, physical tar removal
Sulphur compounds (H_2S, COS)	Corrosion, emissions	Scrubbing (Rectisol), adsorption (ZnO, CuO)

The definition of a gas cleaning system is based on an economic trade-off between gas cleaning and synthesis catalyst performance, i.e. investment in a gas cleaning system versus accepting decreasing performance due to catalyst poisoning [38, 39]. Therefore, the maximum acceptable levels of impurities in the feed gas of fuel synthesis processes are not fixed and may vary from one plant to another. Some indicative syngas specifications for the Fischer-Tropsch and methanol synthesis processes are presented in Table 2-5.

The majority of the world syngas production is achieved by partial oxidation of natural gas [40]. The rest is produced by gasification of coal (SASOL plants, South Africa), while some small amounts are produced in refineries [40]. Since there are no biomass-specific impurities that require a totally different gas cleaning approach, the cleaning and conditioning of the syngas from biomass gasification is quite similar to fossil based syngas (e.g. coal) [39]. This means that it includes cyclons, dust filters, wet-scrubbing techniques (for NH_3 and HCl) and guard beds (ZnO filters) for H_2S.

Table 2-5: FT and methanol synthesis feed gas specifications [36, 38, 39]

Impurity	**Specification**
S (H_2S + COS + CS_2)	< 1 ppmV
N (NH_3 + HCN)	< 1 ppmV
Cl (HCl)	< 10 ppbV
Alkali metals	< 10 ppbV
Solids (soot, dust, ash)	Almost completely removed
Organic compounds (tars)	Not condensing: below dew point
Hetero-organic components (e.g. S, N, O)	< 1 ppmV

2.6.1 Particulates

Particulates originate from the ash in the feedstock, soot (typically from entrained flow gasifiers), and carry-over bed material in the case of fluidised bed gasifiers. Particulates removal apparatus include: cyclones, barrier filters (e.g bag filter), electrostatic filters (ESP) and scrubbers [36, 41].

Cyclones can be used in a wide temperature range but the achieved separation efficiencies are low [36]. By coupling of cyclones (multi-cyclone) higher separation efficiencies can be achieved [41]. Cyclones are more suitable for a first stage separation which is usually followed by barrier filters in order to meet the clean gas requirements. Barrier filters can be designed to separate any particle size and can achieve high particle reduction of 90-99% [36].

Wet electrostatic precipitators also achieve high separation efficiencies and are used for low temperature particulate separation (below 100^{o}C) [36]. They can also partly remove water-soluble gaseous compounds like NH_3, HCl and H_2S [41]. Scrubbers use a scrubbing liquid, in many cases water, to remove particles from a gas stream. Like all wet separation technologies, the gas inlet temperature should be kept below 100°C, which requires gas cooling before the scrubber [41]. Table 2-6 contains a summary of performance of different particle removal apparatuses together with possible operating temperatures.

Table 2-6: Comparison of different particulate separators [36]

Particle removal apparatus	Temperature, ^{o}C	Particle reduction, %
Cyclone	20-900	45-70
Bag filter	150-750	90-99
Wet electrostatic precipitator	40-50	95-99
Scrubber	20-200	40-65

2.6.2 Tars

The major gas cleaning issue in biomass gasification is the presence of tars in the syngas. Tars are condensable organic compounds of high molecular weight with boiling points ranging from 80-350^{o}C [38]. When the temperature in the system decreases to below 350^{o}C, tars start to condense in exit pipes and on filters resulting in blockages and clogged filters and ultimately in system failure [42].

Thermal cracking occurs at temperatures above 800^{o}C [25], with tars being substantially destroyed without a catalyst, usually by addition of steam and oxygen. The effect is similar to direct gasification at high temperature (i.e. an entrained flow gasifier can be used as tar cracker). The main disadvantage of this technology is the production of soot [36].

Catalytic cracking takes place at temperatures of typically 800-900^{o}C using dolomite, nickel-based and other catalysts [5, 36]. A tar conversion rate of over 99% has been achieved by using dolomite and nickel-based catalysts [43]. However, this technology is not yet fully proven and some research and development are still needed [5, 15, 16].

Tars can be also removed by physical removal processes with organic washing liquids. ECN has developed the OLGA tar removal technology which aims at the removal of all aromatic organic components at low temperatures in a scrubber with an oil based medium [38, 40]. In the CHP plant in Guessing, biodiesel is used to clean the syngas to meet gas engine specifications [36]. While appropriate technologies and adequate experience are available, the carbon bound in tars is lost for the fuel synthesis process when physical methods are used [5, 36].

2.6.3 Alkali metal compounds

Alkali metals can damage filters in high temperature and poison synthesis catalysts [25]. They can also damage the gas turbine blades by stripping off their protective oxide layer due to high temperature corrosion [25]. Alkali metal compounds of biomass evaporate during the gasification process. They stay in the vapour phase at high temperatures and therefore pass through particulate removal apparatuses unless the gas is cooled [25]. The maximum temperature that is considered to be effective for condensing alkali metal compounds is 600°C [25]. Tests on alkali metal species have shown that their concentrations in the vapour phase fall with temperature to the extent that concentrations are close to fuel synthesis specifications at temperatures below 500-600°C [44]. Therefore, syngas cooling to this temperature level will cause alkali metal compounds to condense on entrained solids and be removed later on by the particulate separators (see section 2.6.1).

2.6.4 Nitrogen compounds

Nitrogen in biomass mostly forms ammonia (NH_3) and small traces of other nitrogen compounds like hydro cyanide (HCN). These compounds will cause potential emissions problems by forming NO_x if the syngas or the off-gas from the fuel synthesis process is combusted. HCN is highly poisonous for Fischer-Tropsch catalysts and thus it needs to be removed from the syngas.

The common method to remove ammonia from the product gas is scrubbing with a slightly acid liquid, though for low ammonia levels water alone is sufficient [41]. Water scrubbing produces wastewater, which requires extensive wastewater treatment due to the presence of trace contaminants in the gas.

Ammonia and other nitrogen compounds can also be removed by using catalysts like dolomite, nickel, and iron based catalysts, which are also used for tar cracking [41]. As discussed in section 2.6.2, catalytic tar cracking is not a well proven technology and its major disadvantage is the sensitivity of the catalysts in the inorganic impurities of the syngas [36].

2.6.5 Sulphur compounds

Even though biomass only contains minor amounts of sulphur, hydrogen sulphide (H_2S) and carbonyl sulphide (COS) must be thoroughly removed in fuel synthesis plants. The

reason for this is that sulphur is a major catalyst poison as it takes up the active sites of catalysts and reduces the catalytic activity during the reaction, thus drastically reducing performance and the lifetime of common catalysts. Extremely low sulphur contents <1 ppmV are required (see Table 2-5).

Sulphur compounds can be removed by conventional absorption and adsorption processes [36]. To remove sulphur by absorption**,** commonly a basic scrubbing liquid is used, which is a proven state of the art technology [36]. Higher sulphur levels can be conveniently removed by technologies such as Rectisol, Sulfinol, Amisol DEA and MDEA [36]. However, due to their high costs, these methods of removal are only suitable for large scale plants [41].

Adsorption processes are based on the adsorption of the sulphur compounds on a solid material. The most well known adsorbers are based on ZnO or activated carbon and they are widely used in refineries as guard beds [36]. Adsorption processes are generally expensive due to the need for frequent adsorbent renewal and thus are currently used for low sulphur inlet concentrations (normally <50ppm) [36]. Hofbauer et al. [36] provide a thorough and consistent comparison of various absorption and adsorption processes for the removal of sulphur compounds as well as CO_2 from gasification product gas.

2.6.6 Chlorine compounds

Chlorine is another inorganic contaminant which originates from pesticides and herbicides as well as waste wood [25]. At elevated temperatures chlorine causes corrosion of metals and has therefore to be removed [25]. Chlorine can be removed by absorption processes as described in the previous section, or by dissolution in a wet scrubber [25].

2.7 Gas conditioning

The adjustment of syngas composition is known as gas conditioning. In spite of the impurities that cause various problems in a biofuels synthesis plant, the syngas can contain a considerable amount of light hydrocarbons and carbon dioxide that are not harmful but have negative influence on the system performance. These compounds have to be either converted (e.g. CH_4) or removed (CO_2) in order to assure maximum fuel

synthesis yield. Syngas conditioning usually consists of three steps, which are all optional depending on the composition of syngas after cleaning.

2.7.1 Reforming

During gasification, some light hydrocarbons (C_2, C_3) and methane are produced, which can be considered as inert for the synthesis process [5, 36]. Thus, it is necessary to reform these light hydrocarbons from the fuel synthesis step. The chemical energy in these compounds is lost for the fuel synthesis unless they are converted into H_2 and CO in a reformer. The reforming of these hydrocarbons is similar to natural gas based processes and results in higher yields of the FT liquid products [38, 40]. In case of methane, the following reaction occurs in the reformer at temperatures above 800°C [45].

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \qquad \Delta H^{o}_{ref} = +210 \text{ KJmol}^{-1}$$

2.7.2 Water-Gas-Shift

The syngas produced by the gasifier generally has an H_2/CO ratio that ranges between 0.7-1.8, which is lower than the required consumption ratio (H_2/CO = 2) for FT and methanol synthesis [5, 36]. As a result, hydrogen and carbon monoxide are not fully converted and liquid fuels yields are reduced. Thus, the ratio needs to be adjusted by using a water-gas-shift step prior to synthesis. The water-gas-shift reaction takes place in a shift reactor, where CO is converted into H_2 (with steam) at temperatures between 200-300°C.

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad \Delta H^{o}_{WGS} = -41 \text{ KJmol}^{-1}$$

2.7.3 CO_2 removal

Carbon dioxide (CO_2) is considered inert in fuel synthesis processes, therefore it has negative influence on the yield of liquid fuels in the same way as nitrogen. Furthermore, shifting results in an increase of CO_2 concentration in the syngas and this is further aggravated if a recycle loop is used (inert build-up). CO_2 is removed by chemical or physical absorption processes (or a combination of both). For chemical absorption in commercial processes, amines are typically used, while solvents like methanol or polyethylene glycol are used in physical absorption. The CO_2 concentration in the syngas can be reduced to values lower than 0.1 vol% by these processes which can also remove

hydrogen sulphide (H_2S) [36]. Rectisol (Lurgi), Amisol (Lurgi), and Sulfinol (Shell) are examples of commercial CO_2 removal processes (see also section 2.6.5).

2.8 Fuel synthesis

2.8.1 Fischer-Tropsch synthesis

2.8.1.1 Process description

The Fischer-Tropsch reaction was discovered in 1923 by Franz Fischer and Hans Tropsch at the Kaiser Wilhelm Institute for Coal Research in Germany [5, 40]. Fischer-Tropsch (FT) is a process for converting catalytically a mixture of carbon monoxide (CO) and hydrogen (H_2), known as syngas to a variety of organic compounds, including hydrocarbon products of variable chain length. The main mechanism of the FT reaction is:

$$CO + 2H_2 \rightarrow -CH_2- + H_2O \qquad \Delta H^{o}_{FT} = -165\ KJmol^{-1}$$

The methylene group $-CH_2-$ shown in the above equation is used to represent the hydrocarbon chain.

In FT synthesis process, lower temperatures between 200 and 250^{o}C (low temperature Fischer-Tropsch, LTFT) favour the production of liquid fuels up until middle distillates [5, 29]. Contrary to the high temperature Fischer-Tropsch synthesis (HTFT) that operates at 300-350^{o}C, the LTFT synthesis results in lower gas yields to the advantage of higher diesel yields [5, 46] . The FT process is generally operated at pressures ranging from 20-40 bar [5, 16].

There are three main types of FT reactors: fluidised bed, fixed bed and slurry phase reactor. The last two types are considered the most promising according to many authors [5, 15, 16, 29] with some favouring the fixed bed and others the slurry phase reactor. Specifically, an in-house study by Hoek and Kersten [47] showed that the fixed bed reactor will have higher liquids selectivity (or C_{5+} selectivity), lower catalyst consumption and lower CO_2 production compared to the slurry reactor technology. According to Fleisch et al. [48], slurry reactors offer capital cost and operational advantages compared to fixed bed technology. However, they require a unique catalyst/wax separation technology [16, 49].

Iron and cobalt-based catalysts are commercially used for FT synthesis. Cobalt (Co)-based catalysts have a selectivity beyond 90% for the production of alkanes and do not support the water-gas-shift (WGS) reaction [50]. Iron (Fe) catalysts, on the other hand, show a significant WGS activity thus the H_2/CO ratio is adjusted in the FT reactor but result in lower liquids selectivity [5, 50].

Nowadays, FT synthesis is operated commercially by Sasol in South Africa (from coal-derived syngas) and Qatar (from natural gas-derived syngas) [48]. One of the largest implementations of FT synthesis is in Bintulu, Malaysia. This GTL plant is owned by Shell who has recently finished construction on a 140,000 bbl/d GTL plant in Qatar. The plant shipped its first products in 2011 and is expected to reach full production in 2012 [51].

2.8.1.2 Fischer-Tropsch products

Since a wide range of products are obtained from the Fischer-Tropsch synthesis a quantitative approximation of product distributions is necessary. The most widely used approach to tackle this problem is the Anderson–Schulz–Flory (ASF) product distribution. Anderson, Schulz and Flory assumed that during the FT synthesis process, the adsorbed carbon chain can either undergo further addition of a -CH_2- group, or the chain can terminate [52-54]. The ASF-product distribution describes the molar yield in carbon number as:

$$C_n = (1 - \alpha) \cdot \alpha^{n-1}$$

where C_n is the molar fraction of a hydrocarbon product consisting of n carbon atoms and α the chain growth probability, which makes 1 − α the chance that the chain growth terminates. Figure 2-3 shows the hydrocarbon products distribution for different values of chain growth probability α from the Shell Middle Distillate Synthesis (SMDS) process. The liquids selectivity of the process is influenced by a number of factors, such as the type and age of catalyst, the H_2/CO ratio in the feed gas, reactor type and operating conditions [5].

Fischer-Tropsch synthesis results in the production of various products, thus it is not a highly selective process. However, the process offers the possibility to cover the entire range of petrochemical products, thus gasoline, diesel and aviation fuel (kerosene) can be produced with adequate process control. In addition, FT fuels have some outstanding properties, which explain the current interest as a pathway to transport biofuels. They are

high quality and ultra clean fuels, free of sulphur and aromatic compounds [5]. Their major advantage is that unlike other fuels, such as DME and alcohols, they can be easily assimilated in the existing transport infrastructure, both concerning vehicle engines and distribution channels. Table 2-7 shows the specification of FT diesel.

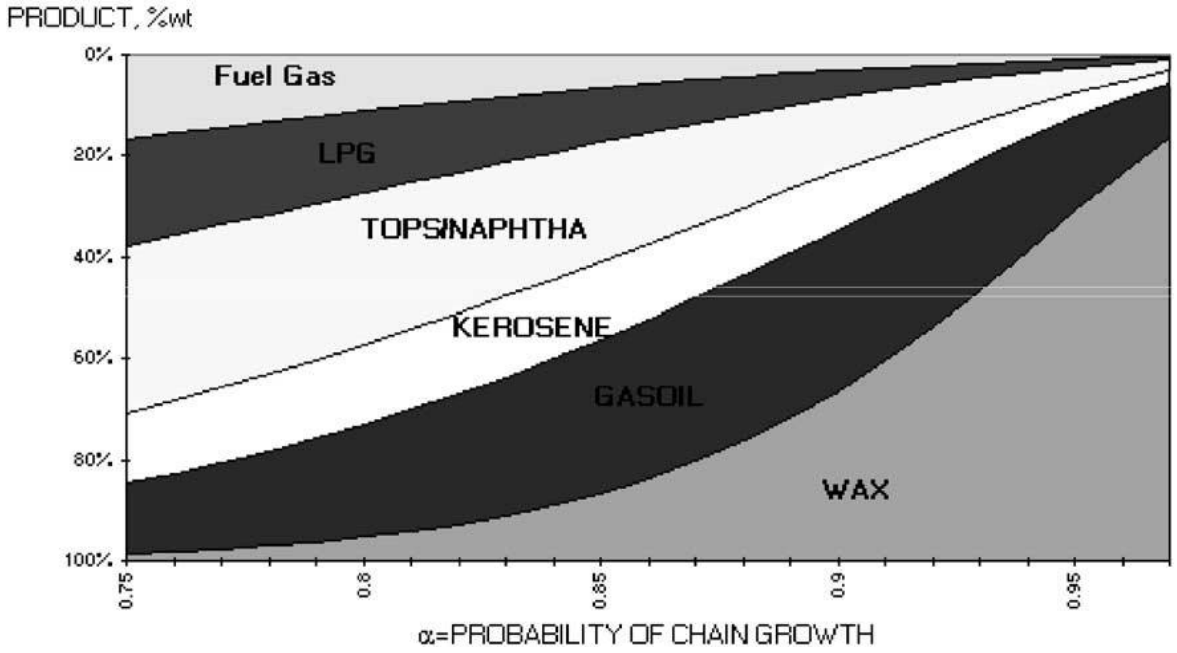

Figure 2-3: Product distribution from Shell Middle Distillate Synthesis Process [49].

Regarding products refining, the lighter FT products (naphtha/gasoline fraction) are separated from the heavier products and isomerised by catalytic reforming to increase its octane number in order to become suitable for blending into conventional gasoline [42].

Table 2-7: Chemical characteristics of FT-diesel with comparison to conventional diesel

Chemical properties	**FT-diesel**	**Conventional diesel**
Lower Heating Value (MJ/l)	34.3 [1] 35.1 [2]	36.4 [1] 35.7 [2]
Density (kg/m^3)	780 [1] 804 [2]	840 [1, 2]
Oxygen content (%wt)	~ 0 [1] 1.6 [2]	~ 0 [1, 2]
Cetane number	50 - 75 [1, 2]	50 [1, 2]
Flash point (^{o}C)	72 [1]	77 [1]

[1][55], [2][42]

The upgrading of the heavier FT products to meet market requirements is achieved by hydrocracking. Depending on the wax cracking conditions, mainly kerosene or diesel are produced as shown in Figure 2-4 [49].

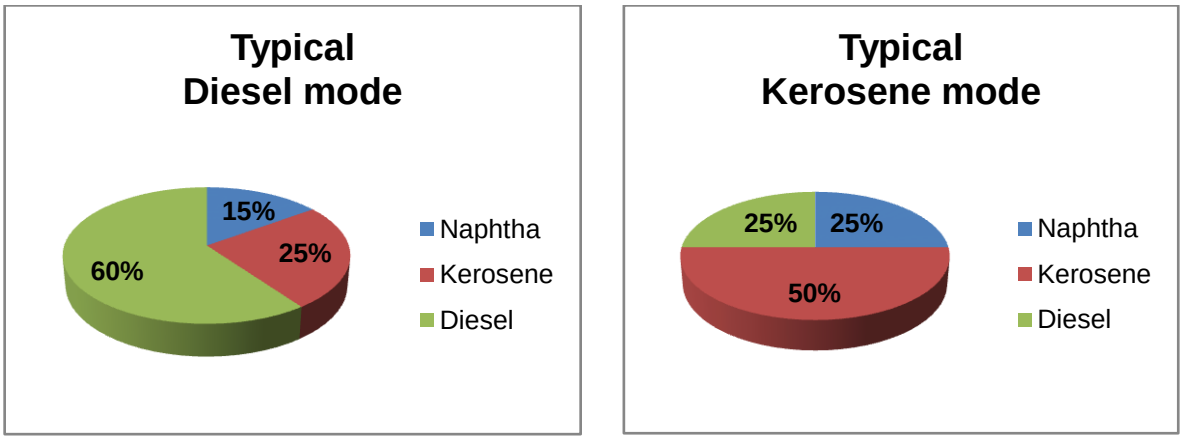

Figure 2-4: Production towards diesel or kerosene

2.8.1.3 Fischer-Tropsch commercial technologies

The two major worldwide manufacturers of liquid fuels by FT synthesis are Sasol (South African Synthetic Oil Ltd.) and Shell:

SASOL

Among the most widely known fuel synthesis plants in the world are the coal-to-liquid (CTL) Fischer-Tropsch plants operated by Sasol in South Africa. Sasol's initial FT reactor technology, the Arge reactor, involved a fixed bed reactor operated at 200 - 250 ^{o}C and 20-30 bar [48, 56]. The Arge reactor primarily produced high boiling hydrocarbons that were used as petrochemical feedstock [56]. This technology was the only FT reactor technology available until the 1950s/1960s when the Sasol Synthol reactors were developed. These were circulating fluidised bed reactors that operated at high temperatures (300-360 ^{o}C) and pressures (20-30 bar). In the late 1990s the Synthol reactors were replaced by the so-called Sasol Advanced Synthol (SAS) reactors [48]. .

The first commercial plant, SASOL I, which came on stream in late 1955 in South Africa included both the Arge and Synthol technology [57]. The SASOL II plant was built on a greenfield site at Secunda by Sasol and commissioned in the early 1980s for the production of liquid fuels and chemicals from coal [57]. The plant relies only on Synthol

reactors since Arge reactors are not included. The SASOL III plant was built by Sasol at its Secunda site in 1982 as an extension to the SASOL II plant in order to increase the production of liquid fuels from coal [57].

The Sasol Slurry Phase Distillate (SSPD) reactor is the latest development of FT reactor technology by Sasol. The synthesis process is carried out in a slurry reactor at 200-250^{o}C and 20-30 bar [48]. The SSPD technology was commercialised on May 1993 in Sasolburg at 2,500 b/d with an iron-based catalyst [48].

Shell

Shell is a worldwide leader in commercial GTL technology with its Fischer-Tropsch plants in Malaysia and Qatar. Instead of using a slurry phase reactor, Shell uses a tubular fixed bed reactor containing a cobalt-based catalyst [48]. The technology applied is referred to as Shell Middle Distillate Synthesis (SMDS) technology, which is normally a three-stage process, as described below [47, 49]:

In the first stage, syngas is obtained by partial oxidation of natural gas with pure oxygen in the Shell Gasification Process, which is a non-catalytic partial oxidation process operated with a flame. The process operates at 1300 to 1500^{o}C and pressures up to 70 bar. The carbon efficiency is in excess of 95%. A Steam Methane Reformer (SMR) is also used to provide the H_2 to compensate for the slight shortage in the hydrogen balance in the HPS stage (2nd stage) and to be used as the feed gas for the HPC stage (3rd stage). The Syngas manufacturing stage is very important not only from a technical point of view but also economically since 50-60% of the process capital cost relates to the sungas manufacturing unit.

In the second stage, known as Heavy Paraffin Synthesis (HPS), the synthesis gas is converted into liquid hydrocarbons via a Fischer-Tropsch (FT) reaction. The multi-tubular fixed bed reactor is filled with a Shell proprietary Fischer-Tropsch cobalt-based catalyst.

In the third and final stage, the crude FT product is fractionated into high-quality products, a part of which is converted into middle distillates by means of the Heavy Paraffin Conversion (HPC), which is a hydrocracking process employing a shell proprietary catalyst and operating typically at 30 - 50 bar and 300 - 350^{o}C. The waxy part of the raw synthesis

product is selectively hydrocracked to the desired middle distillate products. Crucial for the performance is the use of the proprietary hydrocracking catalyst. The HPC product is subsequently fractionated in a conventional distillation column. The product fraction boiling above the gas oil range is recycled to the HPC. Naphtha, middle distillates and waxy raffinate (WR) (low wax content) are produced from the hydrocracked FT product.

2.8.2 Methanol-to-Gasoline (MTG)

The Methanol-To-Gasoline (MTG) process, developed by Mobil (today: ExxonMobil) scientists in the 1970s, was the first major synthetic fuels development in the fifty years since the development of the FT process [58]. A Mobil MTG plant was operated in Motunui, New Zealand from 1985 to 1997 and produced 14,500 bbl/d of unleaded gasoline composed mainly of isoparaffins and aromatics with low benzene content and essentially zero sulphur [18]. The Motunui plant was designed to meet one-third of New Zealand's demand for transport fuels, thus lessening their dependence on fossil fuels import [59]. In 1997, the production of gasoline was abandoned but the plant continued to manufacture methanol. Possible reasons behind this could be the market price of methanol and the crude oil price [18].

In the MTG process, methanol is converted to hydrocarbons and water over zeolite catalysts (ZSM-5). A short description of methanol synthesis, which is the intermediate step of the MTG process, is given in the following section.

2.8.2.1 Methanol Synthesis

Methanol is one of the top ten most produced commodity chemicals and is predominantly produced from syngas which is synthesized via steam reforming of natural gas. The first large-scale commercial methanol plant was introduced by BASF in 1923. The syngas was produced by coal and a water-gas-shift reactor was implemented in the process. The methanol synthesis reactor was operated at temperatures of 300 - 400^{o}C and pressures of 30 - 40 bar, whereas a zinc chromite (ZnO/Cr_2O_3) catalyst was used [60].

Today, methanol is produced by low pressure technology at 200 - 300^{o}C and 50 - 100 bar [60, 61]. The two major worldwide manufactures of methanol are ICI and Lurgi. The ICI low pressure process, which was also used in the MTG process, is shown in Figure 2-5.

Similar to FT synthesis, the methanol reaction requires a consumption H_2/CO ratio of 2 [60, 62].

Methanol is synthesised by the following chemical reactions:

$$CO + 2H_2 \leftrightarrow CH_3OH \qquad \Delta H^{o}_{MeOH} = -90.84\ KJmol^{-1}$$

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \qquad \Delta H^{o}_{MeOH} = -49.6\ KJmol^{-1}$$

In addition, a reverse water-gas-shift reaction occurs over the catalyst:

$$CO_2 + H_2 \leftrightarrow CO + H_2O \qquad \Delta H^{o}_{WGS} = -41\ KJmol^{-1}$$

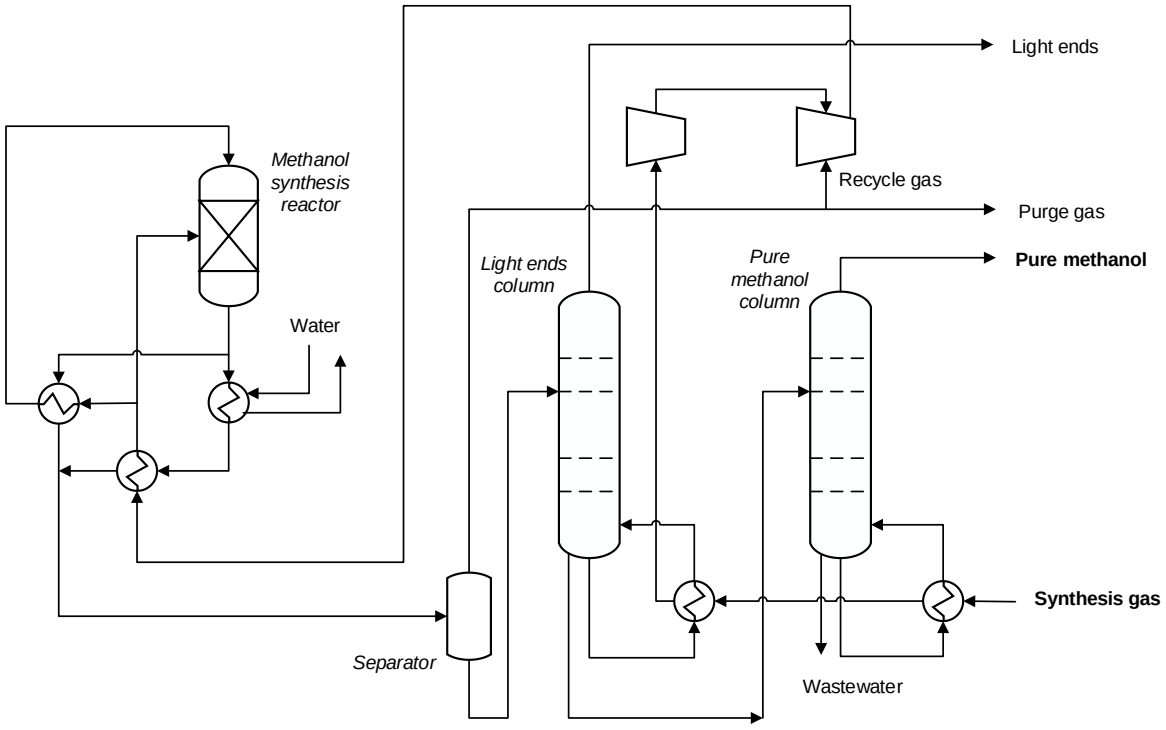

Figure 2-5: The ICI low pressure methanol process

2.8.2.2 The MTG process

During the MTG process, crude methanol is directly converted to hydrocarbons by synthetic zeolite catalysts (ZSM-5). The overall reactions may be represented by the simplified equation:

$$nCH_3OH \rightarrow (CH_2)_n + nH_2O \qquad \Delta H^{o}_{MTG} = -54.4\ KJmol^{-1}$$

where $(CH_2)_n$ represents the average formula of the hydrocarbon mixture produced.

The first step of the MTG process is to pass the methanol over a methanol dehydration catalyst to form a mixture of methanol, DME, and water, and the second step is converting this mixture to gasoline over a zeolite catalyst. Gasoline range compounds (C_5-C_{10}) with no hydrocarbons above C_{10} are produced due to the very selective zeolite (ZSM-5) catalyst [63, 64]. The overall energy efficiency of the Mobil's MTG plant, including the methanol synthesis plant, was 53% [63].

Mobil's MTG plant employed the ICI low pressure methanol process that incorporated two methanol trains, each with a capacity of 2200 t/d [63]. The natural gas was first desulphurised and saturated before entering the reformer reactor, where it reacted with steam over a nickel catalyst at 900^{o}C to produce syngas [64]. The syngas exiting the reformer was sent to the methanol synthesis reactor where it was converted at 250-300^{o}C to methanol and water (17 wt%) [59, 64, 65]. The crude methanol was then sent to the MTG plant for conversion to gasoline compounds.

A simplified block diagram of the MTG process is shown in Figure 2-6. Conversion of crude methanol to gasoline was carried out in two stages [63, 64]: In the first stage, methanol entered a dehydration reactor where it was converted to a mixture of dimethyl ether (DME), methanol and water over an alumina catalyst at 300-420^{o}C. In the second stage, the effluent from the first reactor was mixed with recycle gas from the product separator and passed through the conversion reactors containing the ZSM-5 catalyst, where it was converted at 360-415^{o}C and 22 bar to hydrocarbons and water. The second stage conversion included a system of five fixed-bed reactors in parallel. Methanol was fully converted to approximately 44 wt% hydrocarbons and 56 wt% water [59, 63-65]. Small amounts of CO, CO_2 coke were also formed. After cooling to 25-35^{o}C and condensing, the gasoline product entered the product separator where gas, liquid hydrocarbons and water separated.

After the product separation, liquid hydrocarbons passed to three distillation columns to produce a heavy gasoline stream, a light gasoline stream and a high vapour pressure

gasoline which was used for vapour pressure control [63]. The MTG gasoline contained higher concentration of durene (about 3-6 wt%) than conventional gasoline (about 0.2-0.3 wt%). The concentration of durene in gasoline should be less than 2 wt% to ensure vehicle driveability [65]. Therefore, heavy gasoline was further treated to reduce the amount of durene which could adversely affect product quality.

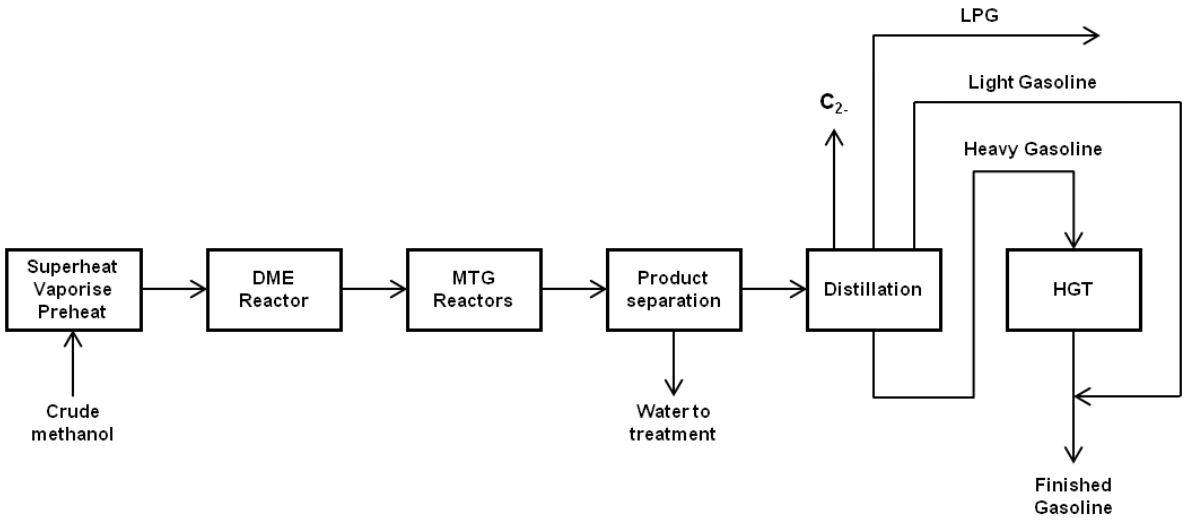

Figure 2-6: Block diagram of Mobil's MTG process

A typical MTG products distribution is shown in Table 2-8. Table 2-9 shows the hydrocarbon compounds composition in gasoline.

Table 2-8: Hydrocarbon products from MTG process [59]

Products	**wt %**
Light gas	1.4
Propane	5.5
Propene	0.2
i-Butane	8.6
n-Butane	3.3
Butenes	1.1
C_5-C_{10} Gasoline	79.9

Since the first MTG plant in New Zealand, ExxonMobil has made improvements in the MTG technology in the early 1990s that reduce both capital investment (by 15-20%) and

operating costs mainly due to reductions in the size and number of heat exchangers [66, 67]. The first coal-to-gasoline MTG plant, utilising the second generation MTG technology, was constructed by Jincheng Anthracite Mining Group (JAMG) in China [66, 67]. The plant started up in June 2009 and its current capacity is 2,500 bpd [68]. Another CTL plant based on MTG technology is planned to be operational in Wyoming, USA towards the end of 2014 with an initial capacity of 15,000-20,000 bpd [66, 67].

Table 2-9: MTG gasoline composition [65]

Compounds	**wt %**
Highly branched alkanes	53
Highly branched alkenes	12
Napthenes (cycloalkanes)	7
Aromatics	28

TransGas Development Systems LLC, has recently begun construction of a coal-to-gasoline MTG plant, the Adams Fork Energy plant in Mingo County, West Virginia. The plant will produce 18,000 bpd of gasoline and is expected to be completed by 2015 [69].

2.8.3 Topsoe Integrated Gasoline Synthesis (TIGAS)

The main principle of the Topsoe integrated gasoline synthesis (TIGAS) is the incorporation of the methanol synthesis and the DME synthesis into a combined methanol and DME synthesis process, thus intermediate methanol production and storage are eliminated. It has been developed by Haldor Topsoe to reduce investment costs and subsequently production costs of gasoline produced from the MTG process [70]. It was demonstrated in Houston Texas where natural gas was used as feed to the process. The demonstration plant of 1 ton/day gasoline started up in early 1984 and terminated in January 1987 after 10,000 hours of operation [70]. A block diagram of the TIGAS process is shown in Figure 2-7.

The aim of this process development work by Haldor Topsoe was to come up with a process scheme in which all three steps of synthetic gasoline production - syngas production, oxygenate synthesis and gasoline synthesis - operate at the same pressure. By combining steam reforming and autothermal reforming for syngas production, and by using a multifunctional catalyst system, producing a mixture of methanol and DME instead

of only methanol, syngas production and oxygenate synthesis can operate at the same relatively low pressure (~25 bar) which eliminates the need for syngas compression prior to synthesis (methanol synthesis operates at 50-100 bar). This results to lower capital costs which are further reduced due to the integration of the methanol synthesis and the DME synthesis into a combined oxygenate synthesis process [70].

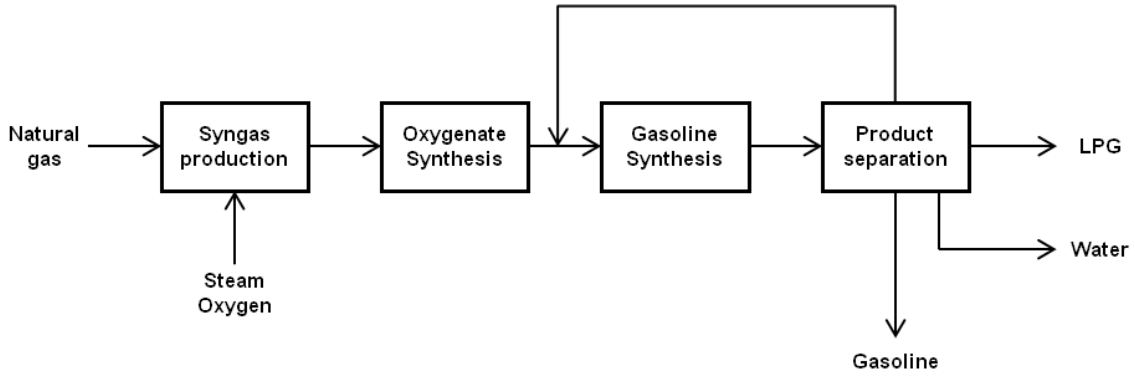

Figure 2-7: Block diagram of the TIGAS process

2.9 Product refining

Refining of the BTL products can be carried out on-site or the crude products can be shipped to a conventional refinery in order to take advantage of established “know-how” and operational experience as well as the economies of scale and an established distribution chain [12].

2.10 Offsites

Offsites are required for all stand alone plants and include power and heat provision, oxygen provision (depending on the gasification method) and waste disposal [12]. Power can be provided on-site for a self-sufficient facility, or it can be partly provided from waste heat from the process. It can also be purchased from the grid. Oxygen can be provided from an on-site oxygen production plant (usually an air separation unit). Significant water amounts will be required for cooling and heating (e.g. heat exchangers). Depending on the process and local requirements, waste disposal and wastewater facilities may be required as well [12].

2.11 Biomass-to-Liquids (BTL) projects

2.11.1 Choren

Choren was one of the leading European companies in the BTL technology based on Fischer-Tropsch synthesis. CHOREN's pilot facility, the Alpha Plant, was constructed in 1997 and had seen 17,000 operating hours by the end of 2004 [71]. Initially constructed for gasification trials, the 1 MW_{th} Carbo-V gasifier, which used forestry wood as feedstock, was complemented with a Fischer-Tropsch reactor in 2002 and thereafter began to produce diesel from for automotive and research purposes [71, 72]. For its FT synthesis technology, Choren used the Shell Middle Distillate Synthesis which employs a cobalt catalyst to recombine carbon and hydrogen into long chain paraffin liquids and waxes (see section 2.8.1.3).

The Choren BTL process, which is shown in Figure 2-8, starts off by feeding biomass into a low temperature gasifier (500^{o}C) to remove volatiles that will form tars at higher temperatures [71].

Figure 2-8: Choren/Shell BTL process

The product gas from the low temperature gasifier passes to the high temperature gasiifer (Carbo-V gasifier) where it is partially oxidised with oxygen and steam at around 1400^{o}C to produce a tar-free gas [71].

The char from the low temperature gasifier is first pulverized, and then blown into the bottom of the high temperature gasifier [71]. The gas that exits the high temperature gasifier is cooled (down to 900^{o}C) due to the endothermic gasification of char, generating steam in the process that is used for power generation [71]. The syngas is then further treated (filtered and scrubbed), and passes to the Fischer-Tropsch synthesis section. The appropriate H_2/CO ratio is set in a shift reactor after which excess CO_2 is eliminated [71]. Choren does not supply any information on the CO_2 removal technology used in their process. The gas composition in three different stages of the process is given in Table 2-10.

Table 2-10: Choren BTL process - syngas composition [71]

Vol.%	**A**	**B**	**C**
CO	36.8	21.8	31.9
H_2	34.6	43.6	64.5
CO_2	22.6	32.5	2.5
N_2	1.7	1.6	0.8
CH_4	0.4	0.3	0.1
H_2O	3.9	0.2	0.2
Sum	100.0	100.0	100.0
A	After gasifier, clean up and compression		
B	After shift reactor		
C	After CO_2 removal		

Previously, the world's first commercial BTL plant was under construction by Choren in Frieberg Saxony. It was initially scheduled to be completed by late 2009 and it would have an output capacity of 15,000 t/yr requiring an estimated 67,500 t/yr of dry biomass (forestry wood and wood residues) [71, 73]. The capital investment was reported to be €100 million [73]. CHOREN was also planning to build large scale plants of 200,000 t/yr of FT diesel the first of which would be in Lubmin on the North-east German coast, to be followed by four additional plants across Germany [73]. However, Choren Industries filed for insolvency in July 2011 because of financial difficulties in starting up the new plant in Frieberg [74]. On February 2012, Choren's biomass gasification technology was sold to Linde Engineering Dresden [74].

2.11.2 NSE Biofuels Oy

NSE Biofuels Oy, which was a joint venture between Neste Oil and Stora Enso, operated a BTL demonstration plant at Stora Enso’s Varkaus pulp and paper mill in Finland from

2009-2011. The output was 656 t/yr of FT fuels from a 12 MW CFB gasifier developed by Foster Wheeller [75]. The CFB gasifier operated with oxygen (40-50%) and steam at atmospheric pressure and 870-890^{o}C [76]. NSE Biofuels (in partnership with Foster Wheeler and VTT) planned to develop a commercial production plant at one of Stora Enso's mills with a projected output capacity of 100,000 t/yr, once enough experience was gained from the demonstration plant [77]. However, in August 2012, Neste Oil and Stora Enso announced that they have decided not to progress with their plans to build a biodiesel plant due to funding being denied from the European Commission [78]. According to Neste Oil, even with public funding, significant investment would also have been required for the commercial plant [78].

2.11.3 BioTfueL project

In 2010, five French partners and Uhde launched BioTfueL, a $113 million project that uses the Fischer-Tropsch process to convert torrified wood biomass into liquid hydrocarbon fuels [79, 80]. The project uses Uhde's proprietary PRENFLO^{TM} gasification process which is an entrained flow gasification technology that operates at 1200-1600^{o}C and 30-40 bar. The PRENFLO^{TM} gasification technology is currently being used in Puertollano, Spain at a 300 MW_e combined cycle power station (the largest in the world) which utilises coal and petroleum coke as feedstock [80, 81]. Demonstrations of using biomass as a supplemental fuel were also conducted in the Puertollano plant [82]. The BioTfueL project is subsidised by €33 million from French Public Funds and includes the construction and operation of two pilot plants in France before moving on to industrial scale production in 2020 [83].

2.11.4 Bioliq project

FZK in partnership with LURGI GmbH is constructing a €60 million pilot BTL plant for biofuel production [84]. The Bioliq process includes decentralised fast pyrolysis of residual straw or wood to produce a pyrolysis bio-oil/char slurry which, according to KIT, its energy density is ten times higher than fresh biomass [84]. The slurry, referred to as biosyncrude, allows for economic long range transportation to a central entrained flow gasification plant for gasoline synthesis via DME using a process similar to TIGAS (see section 2.8.3) [85]. The 2 MW_{th} (0.4 t/h) fast pyrolysis plant is already in operation since 2009 [85]. The 5 MW_{th} gasifier, hot gas cleaning section, and gasoline synthesis section are still under construction with start-up expected in 2012 [85-87].

3 LITERATURE REVIEW OF PREVIOUS BTL TECHNO-ECONOMIC STUDIES

3.1 Introduction

This section carries out a review of the literature on techno-economic studies that have dealt with the production of transport fuels from biomass. The scope of the review has been narrowed to techno-economic assessment studies of biomass gasification and fast pyrolysis systems for production of liquid hydrocarbon fuels, i.e. diesel, gasoline and kerosene. This covers a reasonable number of studies with a high degree of relevance to the present work. The purpose of the review is to place the present study in context and demonstrate its novelty, while also presenting key results from other studies for comparison with those of the present work. It also identifies areas that have not been studied yet and those topics where there was a consensus.

3.2 Previous techno-economic studies

3.2.1 Utrecht University

Utrecht University has been active for many years in the area of bio-energy systems analysis, having conducted a number of techno-economic studies using Aspen Plus for process simulation. Tijmensen et al. [16] carried out a techno-economic assessment of various integrated biomass gasification-Fischer Tropsch (BIG-FT) systems for the production of FT liquids and electricity. In order to cover the wide range of gasification technologies and operating conditions, the study considered five different CFB gasifiers that were available or under development when the paper was written in 2001. Table 3-1 shows the five gasifiers chosen for evaluation in this study.

Table 3-1: Summary of evaluated gasifiers - Tijmensen et al [16]

Gasifier	**Characteristics**		
Battelle Columbus	Atmospheric	indirect	air blown
Termiska Processer	Atmospheric	direct	air blown
Enviro Power	Pressurised	direct	air blown
Gas Technology Institute	Pressurised	direct	oxygen blown
Gas Technology Institute (process adjustments)	Pressurised	direct	oxygen blown

Only CFB gasifiers were selected since the investigated range of thermal input was 100-1600 MW_{th} as CFB gasifiers, along with entrained flow gasifiers, are considered the most suitable gasification technologies for large scale biofuel production. This is further discussed in section 4.5 (see also Table 2-3 at section 2.5.3). Nevertheless, entrained flow gasification was not considered in the analysis. Gas cleaning consisted basically of tar removal and residual contaminations removal. Only the water scrubber was modelled in ASPEN. Tar cracking was not modelled but its capital costs were incuded in the economic analysis. Hot gas cleaning was also considered for evaluation. Gas conditioning included a reformer, a WGS reactor and a Sulfinol process for CO_2 removal.

The selected gasifiers were studied in combination with two different FT-concepts:

1. **Full conversion mode:** In order to maximise the FT liquids production, most of the FT offgas was recycled back to the FT reactor and the remainder passed to a gas turbine.
2. **Once through mode:** The FT offgas was not recycled but passed to the gas turbine where it was co-fired with natural gas for electricity production.

Wood (poplar chips) was used as feedstock. The plant capacity was fixed at 367 MW_{th} LHV_{wet} or 80 dry t/h for all process concepts which were modelled using Aspen Plus. The scope of the study covered all activities from plant gate to product refining. The gasification process was not modelled; instead product gas compositions from literature were used. The authors did not give any explanation for this choice. Biomass preparation (drying, milling) was also not modelled thus the process flowsheet in Aspen begun with the gas cleaning step. Overall energy efficiencies from biomass reception to hydrocarbon biofuel product (LHV basis) were in the range of 33-40% for the atmospheric gasification concepts and 42-50% for the pressurised gasification (22-34 bar) concepts.

Economic analyses were carried out of the various process concepts. 2000 was the base year for the analyses. Total capital costs were estimated at 280-450 million US$ (depending on the concept) using the factored estimation method based on cost data obtained from literature and experts opinion. The FT liquids production costs were calculated by dividing the total annual costs of a modelled concept by the annual produced amount of FT liquids. Production costs of FT liquids were in the range of 13-30 US$/GJ. These included annualised capital repayments, operating and maintenance (including

consumables, labour, waste handling, maintenance), biomass feedstock and electricity supply/demand (fixed power price).

Pressurised gasification concepts resulted in lower production costs. A sensitivity analysis of various key parameters (e.g. capital costs, biomass costs, electricity cost, interest rate) was performed which resulted in a reduction of production costs to 14-16 US$/GJ. By including a number of improvement options (i.e. higher yield, lower feedstock cost, reduction of capital and operating costs through technological learning), production costs could drop to 9 US$/GJ in the longer term.

A second study was carried out by Utrecht University in collaboration with the Energy Research Institute of the Netherlands (ECN). Hamelinck et al [15] using also Aspen for process simulation investigated the performance and costs of various BIG-FT systems for the production of FT liquids and electricity. The scale and type of feedstock remained the same as those of Tijmensen's study above [16].

As with Tijmensen, CFB gasification was the only gasification technology that was considered in the study. However, no information was given on whether the chosen gasifier was modelled based on public data. Contrary to Tijmensen, the Aspen process flowsheet was not provided so comparisons between the two models could not be made. Three different gasification pressure conditions were investigated: 1, 6 and 25 bar. The gasification medium was air, enriched air with oxygen (80%), or pure oxygen.

Gas cleaning included tar cracking and residual contaminants removal. For the FT synthesis, both full conversion and once through options were evaluated as explained in the previously reviewed study. Pressurised (25 bar) oxygen-blown gasification, followed by a tar cracker and wet gas cleaning performed better than other concepts with an energy efficiency of 45% (HHV basis), capital costs at 286 million US$ (2003) and production costs at about 18 US$/GJ (2003). Similar to Tijmensen, pressurised gasification concepts resulted in higher efficiencies than atmospheric gasification concepts. It is not clear if the reported energy efficiency values included also the energy efficiency from electricity production.

As with Tijmensen, the total capital costs were calculated using the factored estimation method based on known costs for major equipment as found in literature or given by experts. Hamelinck also used the same method as Tijmensen to estimate production costs which also included the same cost items (e.g. annualised capital repayment). Production costs of FT liquids were in the range of 18-25 US$/GJ. By assuming a 90% conversion of syngas to FT liquids (70% for the initial concepts investigated) production costs could drop to 16 US$/GJ. However, such a high conversion rate is unrealistic based on the current FT technology which typically achieves 60-70% conversion [5]. In the longer term (larger scale, lower biomass costs, technological learning, and selective catalyst), this could decrease to 9 US$/GJ. These values for short and long term are comparable with the costs found in the previous study by Tijmensen et al. [16] which is not surprising as they were both carried out at the same institute.

A third, more recent study on techno-economics of FT liquid hydrocarbons was published by Utrecht University in 2009 [88]. It is one of the few studies publicly available that not only provides estimates of performance, capital and production costs, but also calculates carbon emissions of 14 FT fuel production plant concepts based on various feedstocks, such as biomass, natural gas, coal or a combination of these. It is also one of the few studies in which the methodology for cost calculations is explained in detail. The main aim of the study was to evaluate which of these 14 FT plant concepts could be economically competitive with fossil-based diesel production plants.

The following biomass feedstocks were considered: forest residues from Canada, eucalyptus from Latin America and willow (or poplar) from Eastern Europe. The authors do not give the reason for choosing these specific feedstocks over others (e.g. energy crops), especially in the case of eucalyptus which is a rather unusual choice compared to other studies.

Table 3-2 summarises the FT diesel production plant concepts evaluated in this study. Pelletisation or torrefaction combined with pelletisation (for TOPs production) were considered as biomass pre-treatment options. Several gasification technologies were evaluated as shown in Table 3-2. These included: fluidised bed gasification, entrained flow gasification and the Carbo-V gasification technology developed by CHOREN. FT synthesis technologies developed by Shell (SMDS) and Sasol (SSPD) were considered for fuel

production. A combination (Adv. FT) of the SSPD process with Shell's HPC hydrocracking process (see section 2.8.1.3) was also considered as promising and included in the study, although such a combination has not been demonstrated yet.

Table 3-2: FT plant concepts studied by van Vliet et al. [88]

	PTL80 SMDS	PTL 400	PTL 2000	PTL 2000 CCS	TTL 2000 CCS	BTL 300 CGP	CTL 400 SPD	CTL 2000	CTL 2000 CCS	GTL 2000 SMDS	GTL 2000	GTL 2000 CCS	XTL 20-80	XTL 50-50 CCS
Feedstock material	FR pellets	Wood pellets	Eucalyp. pellets	Salix pellets	TOPS	Eucalyp. chips	Bituminous coal			ME natural gas			Coal and pellets	Coal and TOPS
Gasifier type[a]	Carbo-V	Carbo-V	Carbo-V	Carbo-V	Shell EF	IGTBFB	Shell EF	Shell EF	Shell EF	PR/SMR	CPO_x	CPO_x	Shell EF Carbo-V	Shell EF
Fischer–Tropsch process[b]	SMDS	Adv. FT	Adv. FT	Adv. FT	Adv. FT	Adv. FT	SPD	Adv. FT	Adv. FT	SMDS	Adv. FT	Adv. FT	Adv. FT	Adv. FT
CCS	No	No	No	Yes	Yes	No	No	No	Yes	No	No	Yes	No	Yes
Scale (MWth in)[c]	80	400	2000	2000	2000	300	400	2000	2000	2000	2000	2000	1595 400	1017 1015

PTL: Pellets-to-Liquids

TTL: TOPs-to-Liquids

Since the study included an assessment of carbon emissions of the selected concepts, carbon capture and storage (CCS) for the resulting CO_2 removed by a Selexol unit was also considered. Mass and energy balances for the selected FT plant concepts were calculated in Excel. There is not sufficient information regarding the structure and the type of the Excel-based models used in this study thus conclusions cannot be made on the reliability of the models. In general, Excel is not usually used for detailed techno-economics studies for the reasons highlighted in section 5.2.1. Therefore, the results of this study should be used with caution.

Energy (biomass-to-fuel) efficiencies for the selected BTL concepts (PTL, TTL, BTL in Table 3-2) were in the range of 48-52%. The FT plant concept based on eucalyptus chips without pre-treatment (BTL 300 in Table 3-2) resulted in the highest efficiency (52%). A pellets-based concept of slightly higher scale (PTL 400) resulted in an energy efficiency of 51%. According to these results, torrefaction and pelletisation does not seem to have an important energy penalty on the overall plant efficiency. However, someone would expect that the effect on the plant efficiency would have been higher due to the thermal pre-processing of biomass by torrefaction and pelletisation. This was not discussed in the study. There is also no information with regards to the heat integration of torrefaction and pelletisation.

Capital costs comprised of installed equipment costs, other direct costs (instrumentation, piping, buildings, etc) and indirect costs (e.g. contingency), although it is not clear what exactly direct and indirect costs included. Equipment costs were estimated using scaling factors. The fuel (diesel) production costs were calculated by dividing the total annual costs of a modelled concept by the annual produced amount of FT hydrocarbons. The total annual costs included annual capital repayments, operating and maintenance, biomass feedstock and revenue from electricity sales and carbon credits. A plant life of 10 years, an interest rate of 10%, operation and maintenance (O&M) costs of 4% of TCI, and a plant availability of 8,000 hours per year were assumed. Labour and fixed costs of 2000 €/$MW_{th,}$ input were assumed in addition to 4% O&M. This assumption was not justified or referenced.

Capital costs for the selected BTL concepts were in the range of 135-1,440 million $€_{2005}$. The BTL 300 concept resulted in capital costs of 273 million $€_{2005}$, whereas the PTL 400 concept resulted in capital costs of 390 million $€_{2005}$. This is mainly due to the additional cost of pelletisation and the more complex gasification technology of the PTL 400 concept.

Production costs for the selected BTL concepts were in the range of 14-25 $€_{2005}$/GJ. The BTL 300 concept resulted in production costs of 15.5 $€_{2005}$/GJ, whereas the PTL 400 concept resulted in production costs of 24.8 $€_{2005}$/GJ, the highest of all concepts. In general, the results of this study showed that pre-treatment of biomass via torrefaction and pelletisation results in higher capital and production costs compared to BTL plants without biomass pre-treatment.

3.2.2 Energy Research Centre of the Netherlands (ECN)

Boerrigter [89] investigated the economics of a BTL plant based on FT synthesis. Process simulation and technical assessment of the BTL plant were not undertaken in this study. The plant efficiency is provided (55%) though no explanation was given on how it was found.

Boerrigter proposed oxygen-blown entrained flow gasification for the plant's gasification technology. This option was identified by the same author [40] as the most suitable for large BTL plants since it has the following advantages:

- High efficiency to syngas

- Fuel flexibility for all types of biomass
- Ability to be scaled-up to a few thousand MW
- It's a well established and commercial technology for coal

For biomass pre-treatment and CO_2 removal, torrefaction and a Rectisol unit were recommended, respectively.

Using a scaling factor of 0.7, the total capital investment (TCI) was estimated for the whole scale range from 10 to 100,000 bbl/d. The GTL plant built by Sasol in Qatar was used as the known scale data (34,000 bbl/d). A depreciation period of 15 years, a required IRR of 12%, operation and maintenance (O&M) costs of 5% of TCI, and a plant availability of 8,000 hours per year were assumed.

It was concluded that the TCI for a BTL plant based on FT synthesis is typically 60% more expensive than a GTL plant with the same capacity. This was due to the 50% higher ASU capacity, the 50% more expensive gasifier due to the solids handling, and the requirement of a Rectisol unit for CO_2 removal. Production costs were in the range of 30 €/GJ (1.1 €/l) for a 50 MW_{th} plant to 15 €/GJ (0.55 €/l) at a scale of 9 GW_{th}. The method for calculating production costs was not explained. It should also be noted that the economic assessment approach followed in this study was relatively simple so results should be looked at with caution.

3.2.3 Vienna University of Technology

In the past decade, several master and PhD-students in Vienna University of Technology developed IPSEpro models that include the entire conversion chain from biomass to electricity generation and district heat. While the commercially available simulation package IPSEpro (see section 5.2) includes a model library for modelling conventional power plant processes, all biomass-related models were specifically developed at the Vienna University of Technology.

These models, along with others that had to be built from scratch (e.g. fast pyrolysis), were used by Fürnsinn [5] who investigated the conversion of woody biomass to FT liquids at small scale (50 MW or approximately 240 dry t/d). This study covers a range of biomass

gasification and FT synthesis concepts and has a high degree of relevance to the present work as these concepts were simulated on IPSEpro.

Various process concepts were identified as particularly promising which were all based on atmospheric steam gasification (as realised in Guessing, Austria). These were evaluated using the process simulation software IPSEpro. The gas cleaning step differentiated between the selected concepts which were divided into “advanced gas cleaning” concepts and a single “starting point” concept. The advanced gas cleaning concepts included a catalytic tar cracker and a CO_2 removal unit (Benfield), whereas the starting point concept was based on the gas cleaning technologies (e.g. physical tar removal) of the CHP-plant in Guessing. The starting point concept included also the co-generation of electricity and heat (polygeneration mode), whereas the advanced gas cleaning concepts were operated either in fuel orientation mode that maximises the FT-liquids yield or in polygeneration mode that produces electricity, FT fuels and district heat. Table 3-3 summarises the biomass gasification and FT synthesis concepts studied by Fürnsinn. Energy efficiencies (LHV basis) were in the range of 49-56% for fuel orientation concepts and 31-43% for polygeneration concepts including the starting point scenario which resulted in the lowest energy efficiency.

Table 3-3: Biomass gasification and Fisher-Tropsch concepts studied by Fürnsinn [5]

Concepts	**Mode**	**Net electricity production (MW)**
FT starting point	Polygeneration	Depending on FT conversion
FT_I	Fuel orientation	< 0 as electricity is bought from the grid
FT_II	Fuel orientation	0
FT_III	Polygeneration	2
FT_IV	Polygeneration	5

Fast pyrolysis for biomass pre-treatment was also considered. Fürnsinn was actually the first to model fast pyrolysis using IPSEpro and some of his models were also used in this study. This is discussed in section 5.5. He investigated three different possibilities in terms of the heat supply for the endothermic pyrolysis reactions. The three fast pyrolysis concepts examined by Fürnsinn are shown in Table 3-4.

Table 3-4: Fast pyrolysis concepts studied by Fürnsinn [5]

Concepts	Pyrolysis heat supply method
Pyrolysis I	Combustion of a part of the produced char. Combustion of permanent gases.
Pyrolysis II	Combustion of a part of the wet (30% moisture) biomass feedstock. Combustion of permanent gases.
Pyrolysis III	Combustion of a part of the dried (10% moisture) biomass feedstock. Combustion of permanent gases.

The first concept gave higher bio-oil yields since all of the available biomass was used to produce bio-oil and the by-product char was used to supply the heat, thus the bio-oil yield was not influenced. For both biomass combustion concepts, the product mix of bio-oil and char contained more char while bio-oil yields were lower. This is due to the fact that a considerable part of the available biomass feedstock (around 10 wt%) was combusted for heat supply, thus less bio-oil was produced. The third fast pyrolysis concept resulted in higher yields of slurry (mix of bio-oil and char). It was chosen, along with the first concept to be examined in connection with the FT_II (see Table 3-3 above) concept which included steam gasification, advanced gas cleaning and FT synthesis. The combination of the fast pyrolysis concepts with the FT_II concept resulted in lower overall efficiencies by 10-20% compared to the solid biomass gasification concepts shown in Table 3-3, due to the thermal pre-processing of biomass by fast pyrolysis.

Fürnsinn also carried out an economic assessment of the modelled concepts which are summarised in Table 3-3 above to estimate production costs of FT fuels. Equipment costs were obtained from the plant manufacturer of the CHP plant in Guessing, although this data is not given in the study. In general, economic calculations are not included and the methodology for the economic assessment is not explained thoroughly. A biomass cost of 83 €/dry t and 7500 h/y of plant operation were assumed. The base year for costing was 2007. For capital costs, values in the range of 40-43 million € were estimated. Production costs were in the range of 0.78-0.93 €/l and included earnings from electricity and district heat depending on the modelled concept. Capital and production costs for the concepts

that included fast pyrolysis as a biomass pre-treatment option were not provided since Fürnsinn did not carry out an economic assessment for these concepts.

3.2.4 National Renewable Energy Laboratory (NREL)

The National Renewable Energy Laboratory (NREL) in the United States have carried out a number of techno-economic studies of biomass gasification and fast pyrolysis systems over recent years, usually considering large scale systems and using Aspen Plus to calculate technical performance.

NREL, in collaboration with Iowa State University and ConocoPhillips, published a report in 2010 that compared two BTL plants based on gasification utilising 2000 dry tonnes per day of corn stover [90]. A scientific paper which summarises the results of this report is also available [91]. The aim was to compare capital and production costs for BTL plants that produce liquid transport fuels and electricity as co-product, using commercially available technology within the next 5–8 years [90].

Two process concepts were analysed. The first concept was based on high temperature (HT) gasification and incorporated a steam/oxygen-fed, entrained flow gasifier (1300^{o}C, 28 bar). The other concept was based on low temperature (LT) gasification which included a pressurized, steam/oxygen-fed fluidized bed gasifier (870^{o}C, 28 bar). Both concepts included FT synthesis for the production of hydrocarbon fuels. Aspen Plus was used for process simulation to calculate mass and energy balances.

In the LT concept, tars were removed by water quenching. This was a rather unrealistic assumption since tars cannot be completely removed by water quenching [36]. Other technologies are more appropriate for tar removal (see section 2.6.2). A WGS reactor was used in both concepts to adjust the H_2/CO molar ratio to the optimal value for FT synthesis. In the HT concept, the WGS unit was placed before the acid gas removal area to allow carbon dioxide produced in the WGS reaction to be removed by the monoethanolamine-based acid gas (CO_2 and H_2S) removal system. In the LT concept, the WGS unit was placed after the syngas cleaning area, right before the FT reactor, due to the presence of tars that have the potential to clog equipment and poison catalysts. However, no information was given on the effect of the increased CO_2 concentration in the

syngas on the subsequent FT synthesis. Other common process steps included biomass preparation, power generation, and cryogenic air separation (for oxygen production).

An economic analysis was carried out for both concepts, assuming the n^{th} production plant (i.e. a plant with technologies that have been used in previous commercial plants). The base year for costing was 2007. Capital costs were based on equipment costs from the Aspen Icarus Process Evaluator software where possible; elsewhere they were capacity factored from equipment costs found in literature. A plant lifetime of 20 years, a required IRR of 10%, biomass cost of 83 $/dry t and a plant availability of 7,446 hours per year (85%) were assumed.

The resulting biomass to fuel energy efficiencies (LHV basis) were 53% and 43% for the HT and LT concept, respectively. For the HT concept, estimated capital costs were approximately 600 million US$, while for the LT scenario they were 500 million US$. The 100 million US$ difference in capital costs was mainly due to the more complex gasifier design for the HT concept. Production costs were approximately 35 $/GJ and 40 $/GJ for the HT and LT concept, respectively.

The majority of techno-economic studies of BTL processes for production of liquid hydrocarbon fuels are based on FT synthesis. Philips et al. [92] decided to take a different approach and conducted a techno-economic study of BTL systems based on the MTG process. This report evaluated the fluidised bed MTG process, in which case direct conversion is possible because, contrary to the fixed bed MTG process, both the conversion of methanol to DME as well as the synthesis of DME to gasoline can be performed in one reactor. The fluidised bed MTG process was also developed by ExxonMobil but it has not been commercialised yet. It was demonstrated in Germany by ExxonMobil and Uhde on a scale of 100 bpd from 1981 to 1984. Details of this project are described by Grimmer et al. [93] and Chang [59].

One concept was evaluated that was based on indirect gasification. Steam was injected to the gasifier from the steam cycle and a char combustor was used to supply heat for the endothermic gasification reactions. Gas cleaning and conditioning consisted of multiple operations: catalytic tar cracking, syngas cooling/quench, WGS and acid gas removal. Detailed mass and energy balance calculations were performed by using Aspen Plus

software. Plant capacity was set at 2000 dry t/d with an expected 8,406 operating hours per year (~96 % plant availability factor). Poplar wood chips delivered at 50% moisture were used as feedstock. Biomass price was 56 $/dry t.

The costs analysis was based on the assumption that this was a n^{th} plant. Thus additional costs for risk financing, longer start-ups, and other costs associated with first-of-a-kind plants were not included. The capital costs were extracted from a variety of sources. For some sub-processes that are well known technologies and can be purchased as modular packages (i.e., amine treatment, acid gas removal), an overall cost for the package unit was used. Investment costs for common equipment items (tanks, pumps, simple heat exchangers) were estimated by using the Aspen Icarus Process Evaluator and Aspen Questimate costing software. For other more specific unit operations (gasifier, LOCAT system), cost estimates from other studies and/or from vendor quotes were used. The base year for costing was 2007.

Capital costs and production costs were 200 million US$ and 0.52 $/l, respectively. These values are low compared to the other BTL studies mentioned here. Overall energy efficiency was 43% (LHV basis) which included energy efficiency from LPG production.

3.2.5 Pacific Northwest National Laboratory (PNNL)

Jones et al. [94] also carried out a techno-economic study of biomass gasification and the MTG process. Two concepts with different gasification technologies were evaluated by using the process simulation software CHEMCAD 6.1. The reason for choosing this software over Aspen Plus or other process simulators was not given. Wood chips (50% moisture) were used as feedstock and the plant capacity was set at 2000 dry ton per day for both concepts.

Biomass gasification was used to differentiate the selected BTL concepts. The first concept was based on a low pressure indirectly-heated gasifier which consisted of two vessels: a gasifier and a char combustor. Steam extracted from the steam cycle is sent to the gasifier which is operated at 870^{o}C and 1.6 bar. The second concept was based on an oxygen/steam-blown fluidised bed gasifier operated at 870^{o}C and 23 bar. A cryogenic air separation unit provides oxygen at 99.5% purity to the gasifier. The dried wood is fed to

the gasifier by using a lock hopper feeder system and pressurized by compressed CO_2 recovered from the CO_2 removal unit.

The indirectly-heated gasifier was modelled using data from a Battelle-Columbus Laboratory (BCL) indirect gasifier. The performance of the oxygen-blown, directly-heated pressurized gasifier was predicted using data from a pressurized, oxygen/steam-blown fluidized bed gasifier developed by Gas Technology Institute (GTI). However, no information was given on exactly what data from BCL or GTI was used to model the gasifiers.

For both concepts, the gas cleaning and conditioning section included a catalytic tar cracker, a water quench, a steam reformer, a LO-CAT oxidation unit for H_2S removal, ZnO beds and an amine-based CO_2 removal unit. No information was given on the type of the amine used in the CO_2 removal unit. The steam reformer was used to convert the methane and other light hydrocarbons to H_2 and CO and adjust the H_2/CO ratio to the optimum value (~2) for methanol synthesis.

The syngas from the CO_2 removal unit was reheated and compressed before entering the methanol synthesis reactor. The methanol synthesis section was based on the low pressure technology (see section 2.8.2.1). Raw methanol at about 95 wt% purity was produced. The MTG section was modelled using data from ExxonMobil's commercialised fixed bed MTG process.

An economic analysis was carried out for both concepts. The base year for costing was 2008. Cost data for the estimation of equipment costs was obtained from literature. The total capital investment is factored from installed equipment costs using the methodology recommended by Peters et al. [95] for solid-liquid chemical plants. A plant lifetime of 20 years, a required IRR of 10%, biomass cost of 66 $/dry t and a plant availability factor of 90% were assumed.

For the indirect gasification concept, estimated capital costs were approximately 383 million US$, while for the direct gasification concept they were 499 million US$. The reported difference in capital costs was mainly due to additional cost for an air separation unit and the more complex gasifier design for the direct gasification concept. Production

costs were approximately 0.70 $/l and 0.80 $/l for the indirect gasification and direct gasification concept, respectively. A sensitivity analysis of capital costs, feedstock price and yield showed that economic viability would require improved yield, reduced capital costs and low feedstock costs (below 20 $/dry t).

Energy efficiencies were 47% and 41% for the indirect gasification and direct gasification concept, respectively. The reported energy efficiencies were calculated on HHV basis and included the energy efficiency from LPG production. Consequently, it is difficult to compare the results of this study with those of most studies mentioned here.

3.2.6 DENA

The Deutsche Energie-Agentur GmbH (DENA) commissioned and published a report in 2006 that compared nine options for production of liquid hydrocarbon fuels based on five processing routes, four of which were additionally considered as integrated into a refinery [96]. Even though only its summary is available, this is one of the few reports publically available that provides a thorough and consistent comparison of various routes to 2nd generation liquid hydrocarbon fuels. Companies and organisations that contributed to this work include: BASF, BP, Choren, FNR, Lurgi, Total and VDA as well as several German Government Departments.

The aim of this project was to develop a basis for the implementation of large scale BTL production in Germany. Nine process concepts were evaluated as summarised in Table 3-5.

No information was given on the fuel synthesis technology that followed the methanol synthesis step, thus it is not known if the MTG process was evaluated in this study. However, it is mentioned that products ranged from 60 to 90% diesel depending on the concept. Therefore, it is very likely that another fuel technology based on methanol synthesis, such as MOGD or Lurgi MtSynfuels, was evaluated.

Processes are understood to be self sufficient in power and heat. Energy crops were used as biomass feedstock. The plant capacity was set at 1 million t/y (wet biomass at 30% moisture thus 700,000 dry t/y or 2400 dry t/d). It is not known how the performance of the

BTL concepts was assessed. The summary does not mention the use of any simulation software.

Table 3-5: The five process concepts studied in the DENA report [96]

	Mechanical treatment	Thermal pretreatment	Gasification	Gas purification	Synthesis	Product conditioning
	d c					
1	Milling		Entrained flow	Gas purification	FT	Product conditioning
		d	c			
2	Shredding	Fast pyrolysis	Entrained flow	Gas purification	FT	Product conditioning
					d	c
3	Shredding		Fluidised bed	Gas purification	Methanol synthesis	Product conditioning
	d	c				
4	Shredding	Pyrolysis	Entrained flow	Gas purification	FT	Product conditioning
	d	c				
5	Shredding	Pyrolysis	Entrained flow	Gas purification	MTG	Product conditioning

d: decentralised; c: centralised

The BTL plants were built on a new location (Greenfield site option) or on a location of an existing refinery. The plant availability for the Greenfield site option was 7000 h/y (80%). Plants built on an existing refinery location resulted in lower capital costs by approximately 25% due to higher plant availability (90%) and lower capital expenditure and operating costs. In general, capital costs were in the range of €400-650 million. The base year for costing was 2006. There were some small inconsistencies on capital costs, such as one large pyrolysis plant (Cases 4 and 5) cost more than several small pyrolysis plants (Case 2), belying the belief in economies of scale. In addition, the advantage of a liquid bio-oil feed to gasification is identifiable in Case 2 (savings of 11 million euros) but this is not apparent in Cases 4 and 5, which were also fed with bio-oil.

Fuel production was between 106,400 and 118,300 t/y hydrocarbons (mass yields of 15% to 17% respectively). Products ranged from 60 to 90% diesel depending on the concept. Case 1 resulted in the lowest production costs (0.88 €/l) in a location with an existing refinery or chemical plant. A sensitivity analysis of biomass price, capital costs and plant

efficiency showed that the cost of production could be lowered to 0.70 €/l. Production costs for the other concepts were not provided.

3.3 Summary of the performance and cost results of the reviewed studies

The performance and cost results of the reviewed techno-economic studies are summarised in Table 3-6 at the end of this chapter. By using the US Chemical Engineering magazine Plant Cost Index, the capital costs in $ were indexed to 2009 which is the costing year of this study (see section 6.2.1). The capital costs in € were indexed to 2009 by using the Engineer magazine International Plant Cost Indices. All capital costs were then adjusted to £2009 using the 2009 annual exchange rate from the Bank of England's web site [97]. They were then scaled to 2016 dry t/d which is the selected scale of this study (see section 4.2) by using the following equation [95, 98]:

$$C_2 = C_1 \cdot \left(\frac{S_2}{S_1}\right)^n \qquad (3\text{-}1)$$

where C_2 is the capital investment of a BTL study reviewed in this section with capacity S_2 (2016 dry t/d) and C_1 is the original reported capital cost of the same study with capacity S_1. The scaling factor n typically ranges from 0.6 to 0.7 [99] thus a generic scaling factor of 0.65 was selected for this study. Scaling the published capital costs to this study's scale allowed for comparison with the capital costs results of this study. This is discussed in section 6.5.1.

Production costs were adjusted to £2009 using exchange rates and inflation rates from the Bank of England's web site. Some studies (Furnsinn, Jones and DENA) provide production costs in $/l or €/l. These were converted to £/GJ by using a volumetric energy density of 34 MJ/l (LHV) and 32 MJ/l (LHV) for FT diesel and MTG gasoline, respectively [100]. Energy efficiencies were given in LHV basis unless otherwise indicated.

The studies reviewed have come from a number of different countries. As a result, there are differences in the units used, feedstock prices, financing assumptions and potential market prices. They also quote prices at different base dates but this was easily dealt with as described above. These studies also differ in scale and the type of hydrocarbons produced, though most of them include the FT process for hydrocarbon synthesis. Table

3-6 is provided below as an indication only of the wide range of performance and costs of different techno-economic studies of BTL plants and a comparison between them should be made with extreme caution (e.g. studies with similar assumptions and methodologies).

Nevertheless, some conclusions can be made:

- Large scale operation (≥ 2000 dry t/d) was considered in most studies.
- The biomass feedstock is usually wood chips from forestry or timber processing.
- Entrained flow and fluidised bed gasification were preferred mainly due to the fact that these two technologies are best suited for large scale operation.
- The most “popular” fuel synthesis process was the FT synthesis process.
- A comparison between BTL concepts based on different fuel synthesis processes (e.g. FT, MTG) was not attempted by any of the studies, with the exception of the DENA report. However, only the summary of this report is available, thus access to important data (e.g. the type of fuel synthesis technology that follows methanol synthesis) is restricted.
- Different operations in the process chain have different degrees of risk and uncertainty. None of the reviewed studies dealt with uncertainty on either performance or costs. Rather than assuming that the input parameters are fixed one should have their model account for uncertainties in the input parameters. An uncertainly analysis was undertaken in this thesis and the methodology is described in section 6.7.

Table 3-6: Performance and cost results of the reviewed techno-economic studies of BTL processes

		Characteristics	Capital costs (million £$_{2009}$)	Capital costs scaled to 2016 dry t/d	Production cost (£$_{2009}$/GJ)	Energy efficiency
Utrecht University	Tijmensen et al. [16]	• 2000 dry t/d • Fluidised bed gasification (oxygen-blown, pressurised) • FT synthesis	322	323	13.8	45%
	Hamelinck et al. [15]	• 2000 dry t/d • Fluidised bed gasification (pressurised) • FT synthesis	237	238	11.8	45% (HHV)
	van Vliet et al. [88]	• 300 MW_{th} (or approx. 1500 dry t/d)* • Fluidised bed gasification (oxygen-blown, pressurised) • FT synthesis	278	337	11.8	52%
ECN	Boerrigter [89]	• 9 GW_{th} (or approx. 43,200 dry t/d)* • Entrained flow gasification • FT synthesis	1,832	250	10.6	55%
Vienna University of Technology	Fürnsinn [5] (average values)	• 50MW_{th} (or approx. 240 dry t/d)* • Steam gasification • FT synthesis • Fuel orientation mode	43	171	17.9	53%
NREL	Swanson et al. [90]	• 2000 dry t/d • Entrained flow gasification • FT synthesis	381	383	18.2	50%
	Swanson et al. [90]	• 2000 dry t/d • Fluidised bed gasification (oxygen-blown, pressurised) • FT synthesis	317	319	20.8	39%
	Philips et al. [92]	• 2000 dry t/d • Steam gasification	127	128	8.5	43%

		• Methanol synthesis and Fluidised MTG				
PNNL	Jones et al. [94]	• 2000 dry t/d • Steam gasification • Methanol synthesis and Fixed MTG	222	223	12	47% (HHV)
	Jones et al. [94]	• 2000 dry t/d • Fluidised bed gasification (oxygen-blown, pressurised) • Methanol synthesis and Fixed MTG	289	291	13.7	41% (HHV)
DENA	DENA 1 [96]	• 2400 dry t/day • Entrained flow gasification • FT synthesis	393	351	22.2	39.8%
	DENA 2 [96]	• 2400 dry t/day • Fast pyrolysis • Entrained flow gasification • FT synthesis	514	459	Not provided	37.2%
	DENA 3 [96]	• 2400 dry t/day • Fluidised bed gasification • Methanol synthesis and subsequent fuel synthesis	618	552	Not provided	36.3%
	DENA 4 [96]	• 2400 dry t/day • Pyrolysis • Entrained flow gasification • FT synthesis	480	428	Not provided	41.3%
	DENA 5 [96]	• 2400 dry t/day • Pyrolysis • Entrained flow gasification • Methanol synthesis and subsequent fuel synthesis	480	428	Not provided	41.3%

* A biomass LHV_{dry} of 18 MJ/kg was assumed.

4 IDENTIFICATION OF SUITABLE OPTIONS

4.1 Introduction

The previous chapters have identified a wide range of technologies, processes and BTL studies for the production of liquid hydrocarbon fuels. This chapter discusses the selection and combination of these technologies to construct BTL process concepts, as well as the rationale behind their selection. The block diagrams included in this chapter outline the necessary process steps (as identified in Chapter 2) in the selected concepts but do not represent complete flow sheets including all process streams. These flow sheets can be found in chapter 5 which is the process simulation chapter.

4.2 Feedstock and plant size

Wood is the feedstock of choice in proposed biofuel systems because of its homogeneity, consistency and quality. Wood has also been and currently is used in commercial bioenergy plants (e.g. Guessing plant, Dynamotive, Varnamo, Choren). There is more information available about wood production, handling and processing than any other biomass feedstock. For these reasons this work focuses exclusively on wood biomass and specifically wood chips since the majority of the studies reviewed in the previous chapter used wood chips as feedstock. The water content and the ash content of the feedstock were arbitrarily set to 30% and 1%, respectively in the modelling to represent typical biomass compositions. The elemental composition of the selected feedstock can be found in section 5.3.2.

According to Bridgwater [101], Dimitriou [102] and other authors [10, 38, 89] large-scale production is generally considered necessary in order to eventually replace a significant proportion of conventional fuels by biofuels. Generally, the preferred scale for biofuels from FT or methanol synthesis with MTG is 2000 dry t/d (approximately 84,000 dry kg/h biomass) (see Table 3-6 at section 3.3). Kilograms per hour (kg/h) is the weight measurement unit for biomass used in IPSEpro, which is the process simulation software used in this study. Therefore, a biomass input of 84,000 dry kg/h (or 2016 dry t/d) was set as the basic plant size for all process concepts. In this study, the term “dry” before weight measurement units accounts for 0% water content in the biomass feedstock. Even though

scale effects on the performance and costs of BTL plants are potentially important, the same scale of biomass input was used for all the selected concepts so that results were directly comparable.

4.3 Feed handling and preparation

Biomass can be transported by road, rail or water. Road transport (trucks) is the typical mode of transport in bioenergy facilities since it offers flexibility and is particularly suited to facilities where the material is transported over distances of less than 100 km [103]. For BTL plants, low cost feedstock is preferred as it results in lower production costs. This usually limits transport distances to less than 100km [104]. Therefore, it was assumed that wood chips are delivered to the plant via trucks [104]. The trucks are weighed as they enter the plant and the wood chips are dumped into a storage pile. From the storage pile, the wood chips are conveyed to a magnetic separator and screened to keep particle sizes within appropriate limits and prevent contamination of the feedstock by metal or rocks. Feed handling and preparation of wood biomass is a well known process as it is already widely practised in the pulp and paper industry. The characteristics and costs of wood chips RSH have been thoroughly investigated by Aston University and specifically by Toft [104] and Rogers [105].

Biomass drying was done by either hot air (rotary dryer) or steam (superheated steam dryer). Air rotary dryers are the most common technology for biomass drying since they are less sensitive to particle size and have bigger capacity compared to other dryers [106]. However, rotary dryers are associated with higher fire risks since they have the longest retention times [106]. Superheated steam dryers (SSD) are less common but are safer that rotary dryers with respect to fire hazard. Since oxygen is not present in superheated steam dryers, the fuel cannot burn, even at elevated temperatures [106, 107]. Fuel synthesis processes, such as FT and MTG generate significant amounts of steam which can be used for other processes within the plant. In this case, superheated steam drying could be preferable. In addition, SSDs do not produce air emissions since all the vapour exiting the dryer is condensed [106, 107]. This, however, means that a wastewater treatment facility will be required [106]. Hot air drying was employed for the fast pyrolysis process and superheated steam drying for the biomass gasification process. This is further discussed in sections 4.4 and 4.5 respectively.

A grinder (hammer mill) is placed after the dryer to reduce the wood chips size to 1mm [24, 90] for the entrained flow gasification concepts. Contrary to entrained flow gasifiers, fluid bed gasifiers are capable of handling a wider variety of biomass particle sizes [23]. Thus no grinding would be required for the concepts based on fluidised bed gasification. The selection of the gasification technologies is further discussed in section 4.5. During drying, light biomass particles can get entrained in the gas flow of the dryer thus significant biomass losses can occur. Consequently, the grinder is placed after the dryer in the feed preparation chain.

It should be noted here that grinding was not modelled on IPSEpro since the simulation software does not allow estimation of particle sizes. It was, however, considered in the economic assessment and its capital and operating costs were included in the cost estimations. Grinding biomass to about 1mm particle size requires a lot of electricity (approx. 0.08 kW_e/kW_{th} wood) [24] which makes this option unattractive for entrained flow gasification.

4.4 Pretreatment

Due the cost of grinding biomass for entrained flow gasification, other pretreatment methods are possible such as fast pyrolysis for liquid production and torrefaction for a grindable solid. Fast pyrolysis was modelled and evaluated as an alternative to grinding for the concepts based on entrained flow gasification. Fast pyrolysis gives a higher energy density liquid that can be transported, handled and gasified more easily than solid biomass, as discussed in section 2.4.1.2. Torrefaction was not considered in this study since this technology is still in early stages of development contrary to fast pyrolysis which has already been commercialised by Dynamotive and Ensyn. Specifically, Ensyn has commissioned a 400 dry t/d fast pyrolysis plant in Alberta, Canada which is expected to be built by 2012 [108]. In addition, research at Bioenergy Research Group (BERG) at Aston University focuses mainly on fast pyrolysis, thus more data necessary for the techno-economic evaluation of this option was available.

The pre-treatment of biomass via fast pyrolysis was assumed to be done in a number of regional fast pyrolysis plants. Each fast pyrolysis plant was assumed to have a capacity of

400 dry t/d [33, 108], thus five fast pyrolysis plants were needed for the BTL plant capacity of 2016 dry t/d selected in this study (see section 4.2). The bio-oil produced from each plant was then transported to a central entrained flow gasification plant for production of hydrocarbon fuels. In the following chapters (5 and 6), the performance and costs of solid biomass and bio-oil for gasification feedstock for BTL are discussed and a comparison is made.

The fast pyrolysis process evaluated in this study was based on a fluidised bed reactor as described in section 2.4.1.1. Fast pyrolysis plants based on fluidised bed reactors have been commercialised by Ensyn (100 t/d wood - plant in Renfrew, Ontario, Canada) and Dynamotive (200 t/d wood - plant in Guelph, Ontario, Canada), thus this is a relatively well tested and proven technology [17, 109].

The fast pyrolysis process included drying, fast pyrolysis of biomass, char separation and combustion for process heat, bio-oil condensation and gas recirculation and combustion for process heat, as shown in Figure 4-1. Drying of biomass was done in an air rotary dryer as discussed in section 4.3.

The heat for drying was provided by the combustion of the non-condensable gases and char, since the plant has to be energetically self-sufficient. This is discussed in detail in section 5.5 in the modelling chapter. In order to supply the necessary heat for the endothermic pyrolysis reactions, either one or any combination of the products, i.e., the permanent gases, the bio-oil, the char or the feedstock must be burnt. Bridgwater [17] provides a comprehensive list of all the methods of providing heat to the pyrolysis reactor. Fürnsinn [5], whose work was reviewed in section 3.2.3, modelled three different options for heat supply to the fast pyrolysis reactor. He showed that the combustion of char and non-condensable gases is a more attractive option in terms of performance and costs than the combustion of biomass (wet or dry) and non-condensable gases. Combustion of biomass results in lower bio-oil yields since part of the available biomass is burnt for heat supply to the reactor. Therefore, in this study, the heat supply option of char (and non-condensable gases) combustion was chosen.

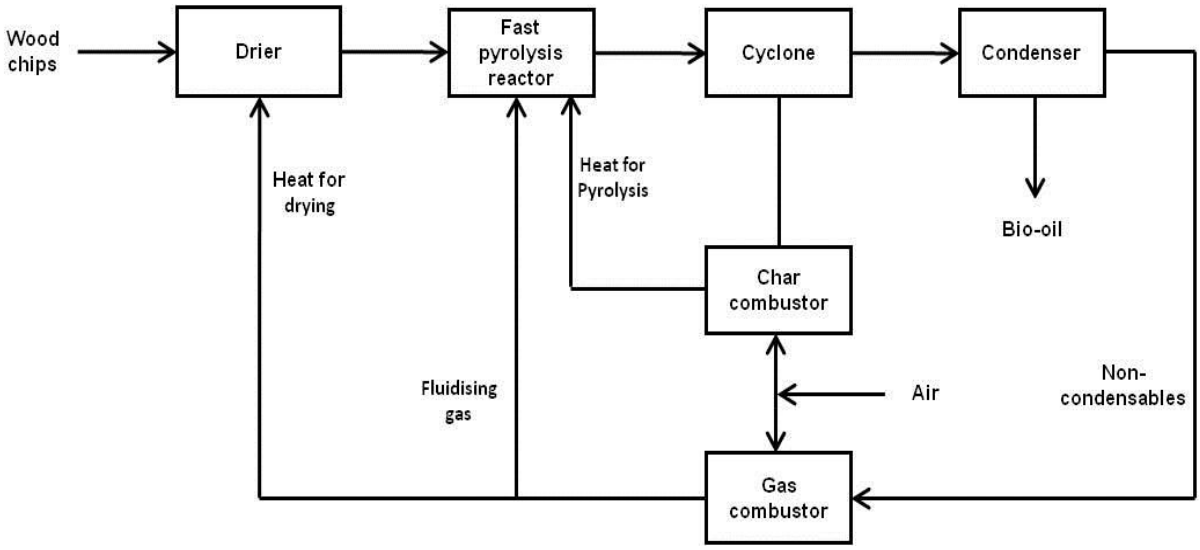

Figure 4-1: Block diagram of the fast pyrolysis concept

4.5 Gasification

As discussed in section 4.2, this study focuses on large-scale production of biofuels. The two gasification technologies best suited for large-scale BTL plants are the circulating fluidised bed (CFB) and entrained flow (EF) gasification [12, 23, 89, 96]. For fluidised bed gasifiers, operating temperature varies between 700-1100^{o}C. CFBs require a large minimum size for viability of typically above 15 t/h dry feed rates and they are relatively easy to scale up from a few MW_{th} to ~100 MW_{th} [23]. Even for capacities above 100 MW_{th}, there is confidence that the industry would be able to provide reliable gasifiers [23]. There is also considerable experience with CFB gasification of biomass (e.g. Varnamo plant, HTW, IGT). Entrained flow reactors are only potentially viable above around 20 dry t/h feed rate and have a good scale-up potential [23]. In addition to its scalability, EF gasification has the advantage that extensive experience is available from coal entrained flow gasification plants (e.g. 2000 t/d coal-fired Shell gasifier in Buggenum, Netherlands) that have been developed to substantial commercial scale units [36, 110]. EF gasifiers can operate at much higher gasification temperatures of up to 1200-1400^{o}C. These high temperatures result in higher carbon conversion, very low tar and methane content and thus lower gas cleaning requirements compared to other gasifiers [24, 89, 91]. Therefore, these two gasification technologies were selected for evaluation in this study.

Both gasifiers were oxygen-blown and pressurised. Many authors, as discussed in Chapter 3, recommend oxygen-blown pressurised gasification for the production of

synthetic hydrocarbon fuels from biomass. Oxygen-blown gasification is preferred to air-blown gasification since in the latter nitrogen acts as an inert diluent, decreasing the efficiency of other processes and necessitating larger (and more costly) equipment. Conversely, oxygen gasification is associated with increased capital costs and energy requirements due to the need for air separation. However, the use of oxygen is usually justified by increased liquid fuels yield due to the higher syngas quality [16, 24, 38, 89, 91]. Capital costs are also decreased due to smaller equipment sizes resulting from the absence of nitrogen.

Pressurised gasification holds the advantage of avoiding a costly compression step before the synthesis process required in atmospheric pressure systems and thus reducing complexity and costs. However, capital and operating costs of such plants can be increased due to the additional costs of building pressure vessels [23]. These additional costs are to some extent balanced by savings from reduced piping sizes, the avoidance of gas compressors for the synthesis reactor and higher efficiencies [23]. The circulating fluid bed demonstration plant at Värnamo in Sweden, which was built and operated by Foster Wheeler and Sydkraft is an example of pressurised gasification.

Biomass feeding for pressurised gasifiers is a technology area where additional development is needed. Lock hoppers are the conventional pressurising technology for coal-fired gasifiers. The main drawback of this pressurised feed system is the high requirements of inert gas (usually N_2 or recovered carbon dioxide) and the additional costs of the inert gas compression [24, 111]. A number of efforts have been made to develop alternative pressurised feed systems to address the disadvantages of lock hoppers. These include rotary, screw, piston and screw/piston feeders [111]. None of these have yet been demonstrated in large-scale operations [111].

At the demonstration plant at Värnamo, the preconditioned feedstock was pressurised in a lock hopper system by N_2 before being passed to a CFB gasifier via a pressurised vessel [112]. This is maybe affordable in a small-scale facility, such as the Värnamo plant, with limited operation time. However, in a large-scale commercial plant this will be far too expensive and needs to be solved in another way [113]. Therefore, it was decided to use CO_2 as the pressurisation gas which was acquired from the downstream CO_2 removal unit.

This way nitrogen dilution in downstream equipment is also avoided. The use of CO_2 as pressurisation medium is also proposed by Swanson [91], Larson [114] and van Drift [24].

Air drying of biomass is not desirable for large-scale operations due to the high risk of fire. Therefore, superheated steam drying was employed for both gasifiers. Another reason behind this selection was that FT and MTG generate significant amounts of steam which can be used in other parts of the plant, such as the dryer [114]. More information on the operating conditions, syngas composition, etc, is given in the next chapter where the simulation of the selected concepts using IPSEpro is discussed.

4.6 Gas cleaning & conditioning

Gas cleaning is considered to be one of the biggest challenges to the development of a successful BTL plant. The impurities in syngas need to be reduced to the level demanded by the catalytic fuel synthesis processes, as discussed in section 2.6. For each plant, and also for each type of catalyst, the acceptable levels of contaminants may be different. Even though it is claimed that there are no insuperable problems associated with cleaning of biomass-based syngas, there is no large scale or long term experience.

Tars are the major gas cleaning issue in biomass gasification, as discussed in section 2.6.2. For the CFB concepts, a catalytic autothermal steam reformer was employed for tar destruction, as well as reforming of light hydrocarbons and ammonia [115]. A tar cracker was not necessary for the EF concepts due to the high operating temperature of the gasifier (1400^{o}C) that inhibits tar formation.

Catalytic tar cracking is recommended by many authors [5, 15, 16, 94, 116], even though this technology has not yet been demonstrated on large-scale. However, there is a significant ongoing research on tar reforming catalysts, especially on dolomite and nickel-based catalysts. Specifically, at the Varnamo plant, 95-99 % of tars in gas streams were successfully cracked in a catalytic (dolomite catalyst) cracker at 750-900^{o}C under laboratory conditions [117]. Other catalysts also have been proved effective at tar decomposition. Pfeifer achieved an almost complete tar destruction (approx. 98%) and considerable ammonia decomposition (approx. 40%) using commercial steam reforming nickel catalysts at temperatures above 850^{o}C [118]. These catalysts were tested in a

laboratory scale reactor fed by slip streams taken from the dual fluidised bed steam gasifier plant in Güssing, Austria. Caballero [119] and Aznar [120] also reported that 98% of tars, 87-99% of methane and 100% of other light hydrocarbons in raw syngas streams were successfully reformed at 780-830^{o}C using commercial nickel-based catalysts (e.g. BASF, Haldor Topsoe). The experiments took place in a laboratory scale reactor fed by raw syngas from a 5-20 kg wet biomass/h fluidised bed steam/oxygen blown gasifier [119, 120].

Filters and cyclones were employed for the removal of particulates and alkali compounds (see section 2.6). For the EF concepts, a water quench was placed after the gasifier for removal of particulates and syngas cooling. This was also proposed by several authors [40, 90, 92, 94]. For the CFB gasifier, cooling of syngas was done by a heat exchanger to use the generated steam for tar cracking/reforming. A water quench is also used to remove ammonia from the syngas but for gasifiers coupled with a tar reformer, such as the CFB gasifier in this study, most of nitrogen compounds can be cracked in the tar reformer, thus a water quench was not employed for the CFB concepts.

Sulphur in the biomass mostly forms hydrogen sulphide (H_2S) with small amounts of carbonyl sulphide (COS). A Rectisol unit was assumed for the removal of sulphur species, as well as CO_2. Rectisol is a very efficient process for the removal of the acid compounds since the achieved concentration of CO_2 and H_2S could be as low as 2 ppm and 0.1 ppm respectively [36]. In addition, it has been proven successful in large scale applications. Rectisol was also chosen due to data availability, as compared to other large scale acid gas removal processes, such as Amisol and Sulfinol. The low nitrogen, chloride and sulphur concentrations in the raw biomass syngas from oxygen-blown gasifiers ensure that the resulting HCN, NO_x and SO_2 emissions are well below permitted levels for the downstream fuel synthesis process. Nevertheless, Rectisol can also remove trace components, such as HCN and HCl [36].

The simulation of the EF concept on IPSE showed that the H_2/CO molar ratio of the dust free syngas was lower than the required ratio (H_2/CO = 2) for FT and methanol synthesis. Therefore, the ratio was adjusted by using a water-gas-shift (WGS) reactor. The WGS unit here allowed carbon dioxide produced in the reaction to be removed soon after in the Rectisol unit. Simulation of the CFB concept also showed that a WGS unit was not

necessary for the CFB-based concepts since the H_2/CO ratio of the syngas exiting the tar cracker was approximately 2. This is mainly due to the fact that light hydrocarbons and tars are almost fully reformed in the tar cracker/reformer. This also depends on the composition of the raw syngas from the gasifier. EF gasifiers produce syngas with high concentrations of hydrogen and carbon monoxide due to the high conversion of tars and light hydrocarbons. This results in lower H_2/CO ratios compared to fluidised bed gasifiers. The CFB and EF gasification concepts with their downstream gas clean-up configurations are shown in Figure 4-2 and Figure 4-3, respectively.

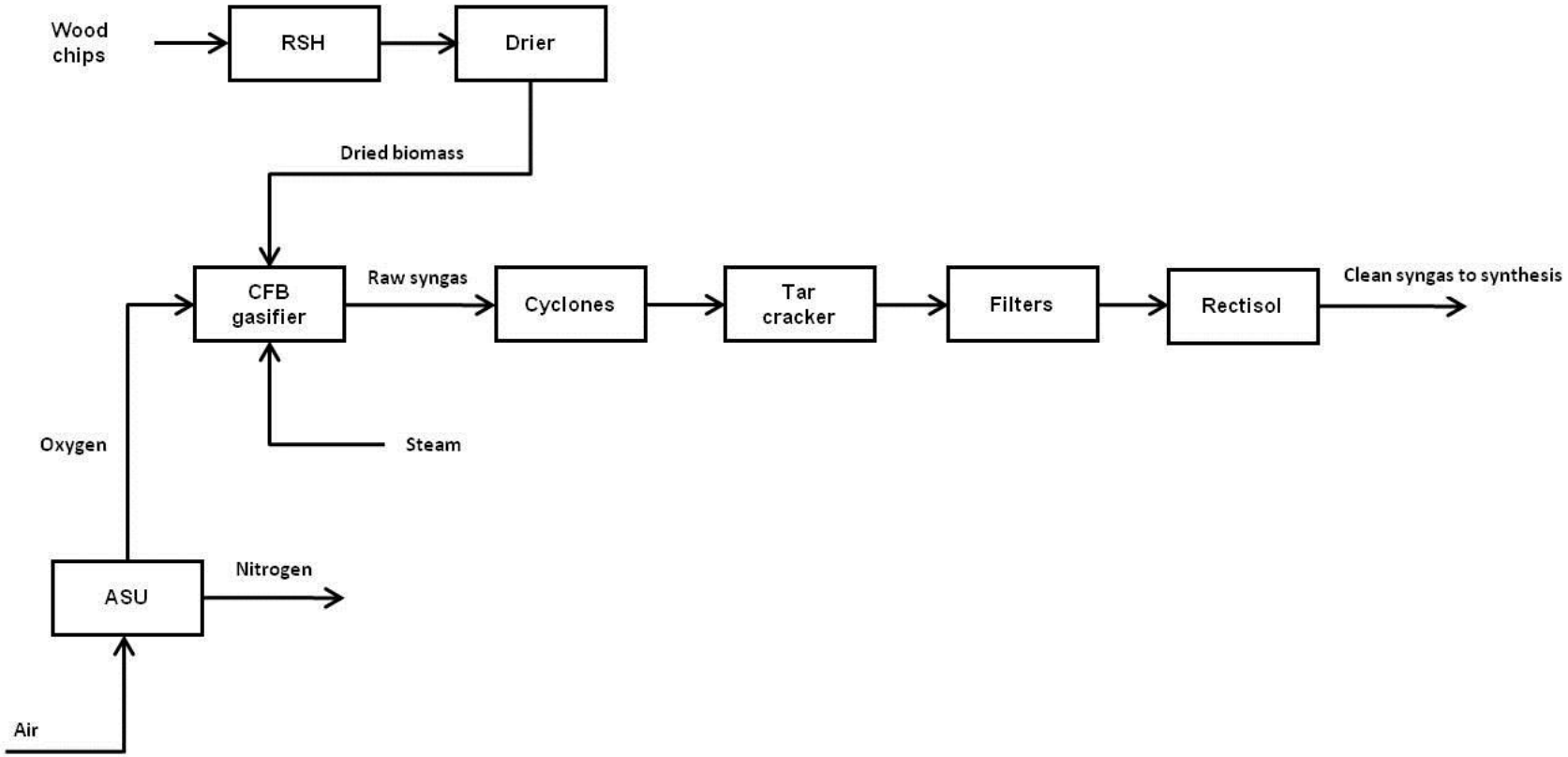

Figure 4-2: Block flow diagram of the circulating fluidised bed (CFB) gasification concept

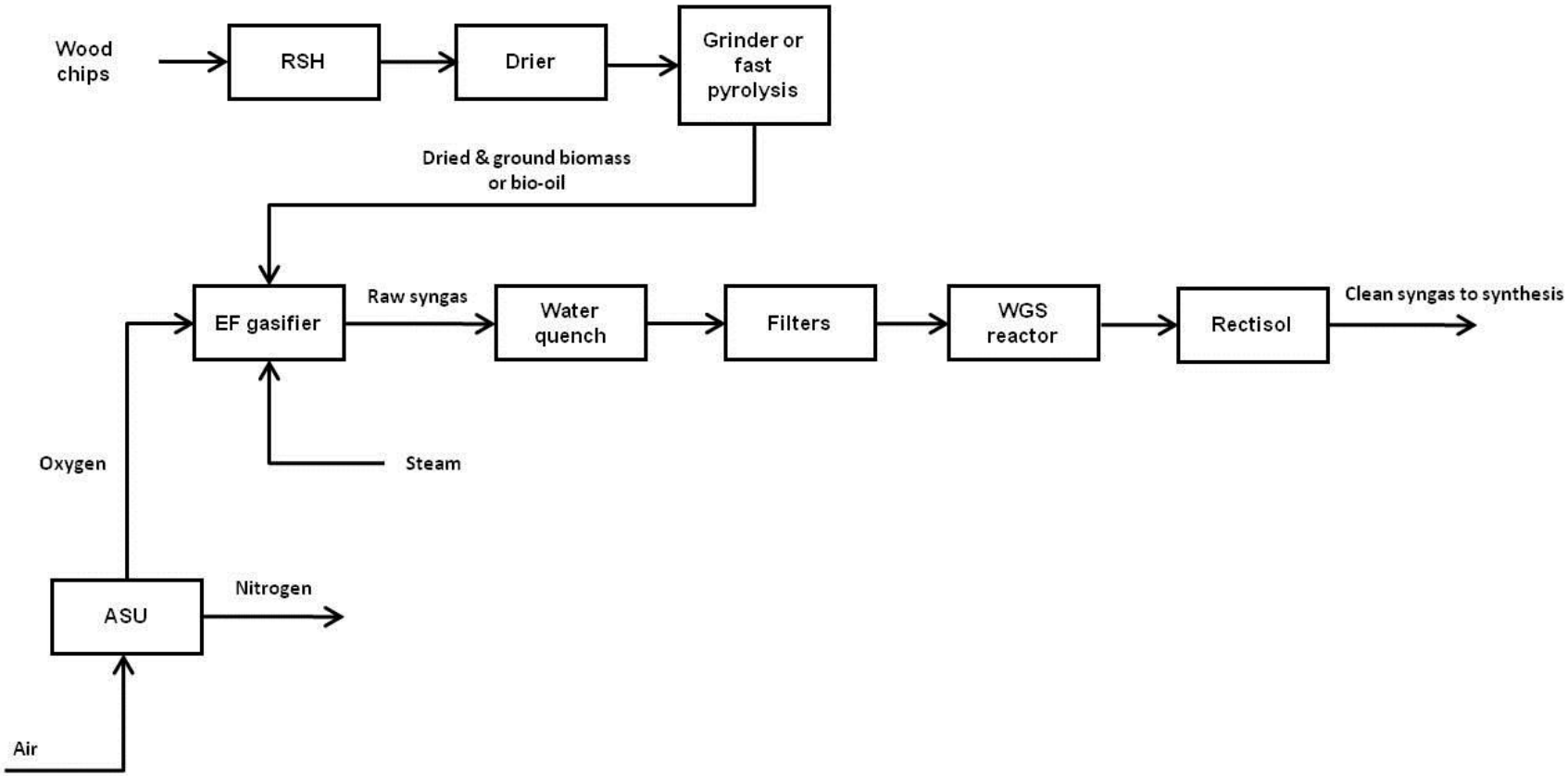

Figure 4-3: Block flow diagram of the entrained flow (EF) gasification concept

4.7 Fuel synthesis

Liquid transport fuels were produced from syngas using either FT synthesis, methanol synthesis followed by the MTG process or the TIGAS process:

- FT synthesis was chosen since it has already been used in large-scale CTL and GTL plants throughout the world, as discussed in section 2.8.1.3.
- The production of methanol from natural gas has also been proven successful in large scale applications (e.g. ICI, Lurgi). The synthesis of fuels from methanol via the MTG process has also been commercialised by ExxonMobil in 1980s in New Zealand.
- Even though there is very limited available data on the demonstration TIGAS plant developed by Haldor Topsoe, it was decided to evaluate this process to compare it with the MTG process. As discussed in section 2.8.3, the TIGAS process can result in lower capital costs compared to the MTG process by avoiding a costly syngas compression prior to methanol synthesis, as well as due to the integration of the methanol synthesis and the DME synthesis into a combined oxygenate synthesis process. Extensive efforts were made to acquire performance and cost data for the TIGAS process from various contacts at Haldor Topsoe but without success.

Simplified block flow diagrams of FT synthesis, MTG and TIGAS are shown in Figure 4-4, Figure 4-5 and Figure 4-6, respectively.

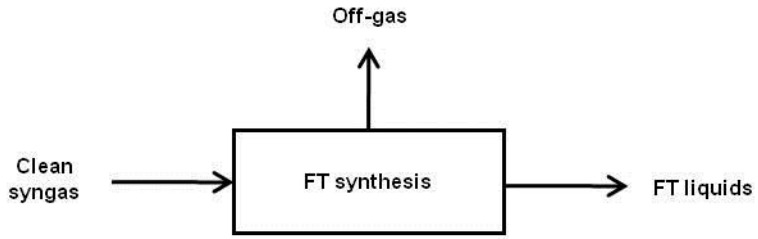

Figure 4-4: Block flow diagram of FT synthesis

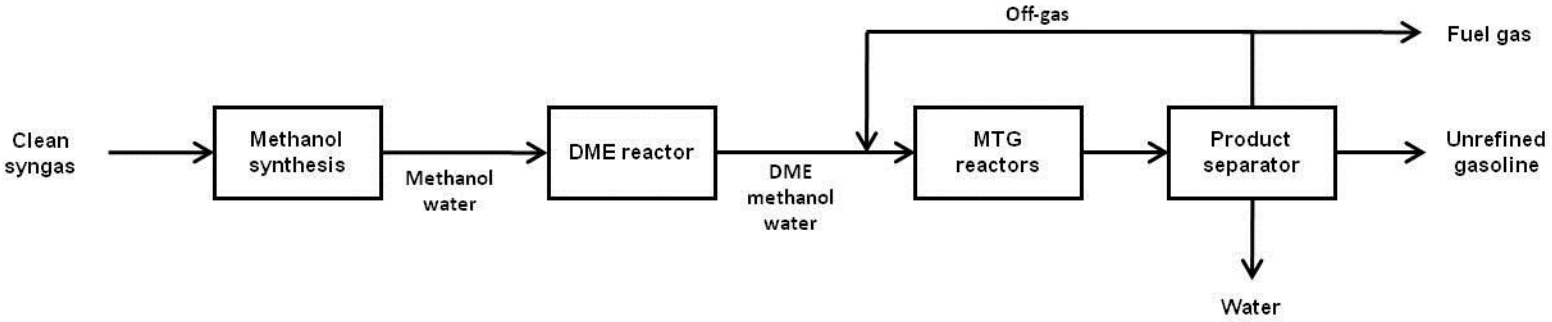

Figure 4-5: Block flow diagram of methanol synthesis and MTG

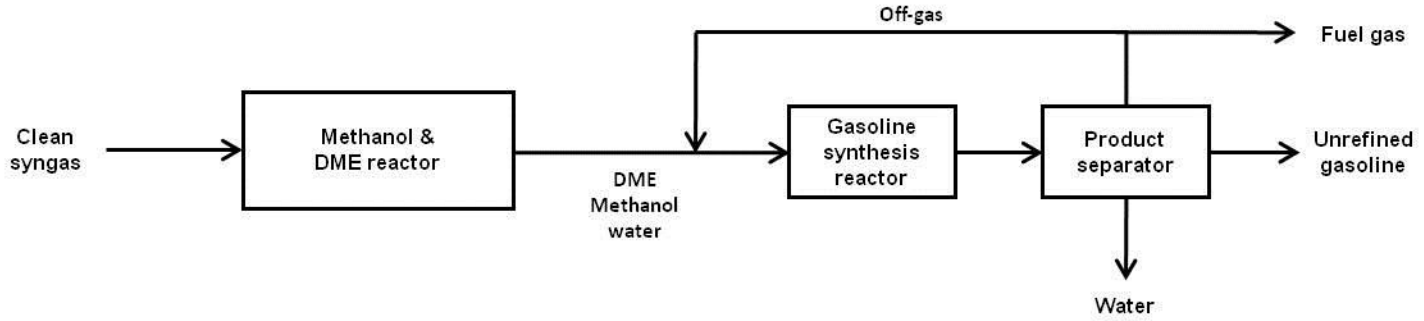

Figure 4-6: Block flow diagram of TIGAS

4.8 Utilities

A cryogenic air separation unit (ASU) was employed to supply the oxygen to the gasifiers since cryogenic distillation has been the predominant air separation technology for large-scale operations for over 75 years [121]. It can account for up to 15% of the total gasification plant cost and is an energy intensive process [121]. Other technologies include ceramic ion-transfer membranes (ITM) and pressure swing absorption (PSA) which are not mature technologies [121], thus they were not considered in this study.

Synfuels plants typically include a power island for heat balancing and to generate electricity for both internal use and export. A power plant was not modelled on IPSEpro due to time constraints and to avoid complexity. It was, however, considered in the economic assessment and its capital and operating costs were included in the cost estimations.

4.9 Selected process concepts

The BTL process concepts selected for techno-economic and uncertainty assessment are summarised in Table 4-1.

Table 4-1: The BTL process concepts analysed in the study

BTL concept	Preparation	Pre-treatment	Gasification	Gas clean-up	Fuel synthesis	Fuel product
EF-FT	SSD dryer, grinder		Entrained flow	Gas clean-up as shown in Fig. 4.3	Fischer-Tropsch	Diesel, gasoline, kerosene
EF-MTG	SSD dryer, grinder		Entrained flow	Gas clean-up as shown in Fig. 4.3	Methanol synthesis followed by MTG	Gasoline
EF-TIG	SSD dryer, grinder		Entrained flow	Gas clean-up as shown in Fig. 4.3	TIGAS	Gasoline
CFB-FT	SSD dryer		Circulating Fluidised bed	Gas clean-up as shown in Fig. 4.2	Fischer-Tropsch	Diesel, gasoline, kerosene
CFB-MTG	SSD dryer		Circulating Fluidised bed	Gas clean-up as shown in Fig. 4.2	Methanol synthesis followed by MTG	Gasoline
CFB-TIG	SSD dryer		Circulating Fluidised bed	Gas clean-up as shown in Fig. 4.2	TIGAS	Gasoline
FP-FT	Air dryer, grinder	Fast pyrolysis	Entrained flow	Gas clean-up as shown in Fig. 4.3	Fischer-Tropsch	Diesel, gasoline, kerosene
FP-MTG	Air dryer, grinder	Fast pyrolysis	Entrained flow	Gas clean-up as shown in Fig. 4.3	Methanol synthesis followed by MTG	Gasoline
FP-TIG	Air dryer, grinder	Fast pyrolysis	Entrained flow	Gas clean-up as shown in Fig. 4.3	TIGAS	Gasoline

5 PROCESS SIMULATION

5.1 Introduction

Computer programs for process simulation can be divided into dynamic and stationary tools [122]. In dynamic simulation, variations of process parameters with time are analyzed allowing the prediction and control of chemical processes in real time. However, dynamic simulations are characterised by increased calculation times and are more complex than stationary simulations [95]. Stationary programs can be used for the analysis of steady-state operations, i.e. without any variations of parameters over time [95]. They are particularly useful for mass and energy balances calculations, as well as investigating long-term equipment performance. Therefore, they provide a reasonably good estimate for process equipment and raw materials needs and utility requirements [95].

The modelling task of this techno-economic study is the development of a steady-state representation of various BTL process concepts which were discussed in the previous chapter. The purpose is to calculate mass and energy balances and thus overall efficiencies for each process concept to enable costs estimations and comparisons of the selected BTL concepts.

Steady-state processes are modelled as a network of conversion units interconnected by process streams. Process units typically include chemical reactors, stream splitters, heat exchangers, pumps and turbines, which are mathematically modelled by mass and energy balances and by thermodynamic principles [41].

Stationary simulation programs differ in various aspects but share some common characteristics such as model libraries for unit operations and user interfaces that are based on flow sheets. However based on the way the results are calculated, stationary simulation programs can be divided into sequential-modular and simultaneous or equation oriented simulation programs [5, 41].

In sequential-modular simulation programs, the entire flow sheet is calculated by solving the units in the same order as they appear in the process. An equation solver is run locally for each unit before the system proceeds to the next. Thus, the results of the first unit

represent the input data for the second, and so on. As a result, the calculation path can be easily followed and thus assisting with the localisation of errors. However, complex systems that include a large number of recycled streams usually lead to long calculation times [41]. Aspen Plus is an example of a sequential-modular process simulation program.

In contrast, in simultaneous or equation oriented simulation programs the flow sheet is translated into an equation system containing the same number of equations as variables. This system is then solved in one step, regardless whether input or output parameters of a unit are defined, resulting in short calculation times. Any parameters can be specified as long as they are independent of each other. Flexibility is thus maximized and even large complex systems can be calculated [5, 41, 123]. However, the calculation path is not so easy to follow, thus locating errors becomes more difficult than for sequential-modular calculation [41, 123]. IPSEpro is an example of an equation oriented simulation program.

The main differences between the two simulation approaches described above are summarized in Table 5-1 below.

Table 5-1: Comparison of stationary computer simulation programs

Type	**Advantages**	**Disadvantages**
Sequential-modular	Detailed description of single units.	Long calculation times and instabilities for large and strongly linked sheets.
Simultaneous or equation oriented	High flexibility and short calculation times make it appropriate for complex flow sheets.	Difficult localisation and identification of errors.

5.2 Process simulation with IPSEpro

5.2.1 Why IPSEpro?

The literature review in Chapter 3 revealed two main modelling approaches to studies of this kind. In one, a process simulation software is used, typically Aspen Plus, usually to resolve complex configurations. This generally requires a process simulation program to be already available since few studies of this kind would have the time and resources to

develop their own. In the other, which is the least preferred one, Microsoft Excel spreadsheets are used.

The high level of flexibility which equation oriented programs like IPSEpro offer is particularly suitable for process comparisons as required in this study because complete processes can be compiled from sequences of units that are simply described in terms of inputs and outputs. The relationships and parameters between units can be readily modified to account for new information or changed conditions. The more sophisticated Aspen approach requires a more detailed flowsheet in which each component is considered individually. This reduces the flexibility of complex process configurations and leads to iteration difficulties as described above.

Microsoft Excel, on the other hand, requires more complex constructions to enable process modules to properly interact, and while innately simpler requires much more effort to construct a suitable and versatile model.

IPSEpro is an example of an equation oriented process simulation environment which is licenced by SimTech Simulation Technology, an Austrian company located in Graz. Apart from short calculation times (typically less than a second) and high flexibility in terms of parameters settings, IPSEpro holds the following additional advantages compared to Aspen and Microsoft Excel [5, 41, 123]:

- High level user-friendly graphical interface and ease of operation. The level of detailed knowledge needed and the amount of possible changes can easily be adjusted to the users performing the calculations as well as to the simulation task.
- It allows the creation and implementation of user defined model libraries which contain all the information about the process units and streams.
- It has an extensive database of physical and chemical properties associated with thermo-chemical conversion processes. It also allows the creation of new property databases or alterations of the existing ones. This is of specific importance for the effective implementation of new technologies, such as biomass gasification and fast pyrolysis.
- Good support and individual attention offered by the software developer. SimTech is a relatively small company and thus it is easier to be contacted when technical support is needed.

- Good collaboration with Vienna University of Technology who developed the model library used in this study. Further details about the library are given in the next section.

5.2.2 IPSEpro structure

IPSEpro was designed in a modular structure as shown in Figure 5-1 [124]. The Process Simulation Environment (PSE) is the user interface where the process is modelled and data is entered. IPSEpro models are mathematical descriptions of the behaviour of process units (or component models) in terms of equations (e.g. energy balance equations) and other items like variables and parameters. Setting up the mathematical model of the process in PSE means to combine the equations and variables of all component models into one single system. PSE does this automatically while the user connects component models on the flow sheet.

When a calculation is performed, data from the PSE is sent to the equation solver (Kernel), which refers to a model library that contains the information about the units used in the process. The model library can be edited by the user with a special editor, the Model Development Kit (MDK), which is a separate module of the IPSEpro package. MDK provides a Model Description Language (MDL) that allows users to describe their models mathematically, once their equations are identified. An example of an IPSEpro model (dryer) on the MDK is given in Appendix A.

The concept of MDL is very different from the one used in traditional programming languages like FORTRAN, Pascal or C++. These traditional languages are based on a sequential concept: statements are processed sequentially, as they appear in the code [124]. This sequence is frequently interrupted by control statements. However, the main flow of the program is sequential. MDL is an equation-oriented language. A model is defined by writing a system of equations. The sequence of the equations has no influence on how the equations are processed.

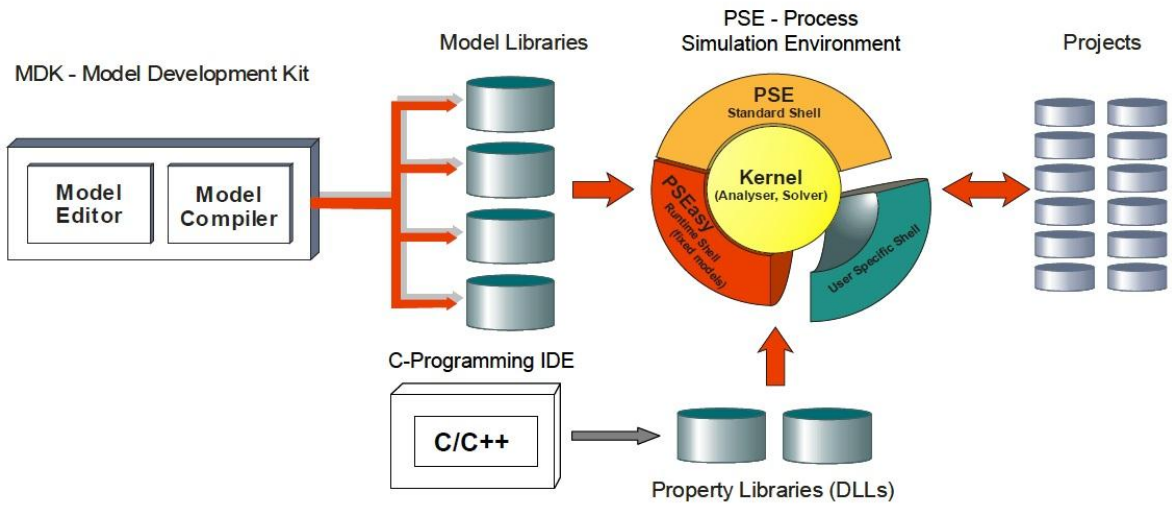

Figure 5-1: Modular structure of the process simulation software IPSEpro

Thermodynamic property data, i.e. functions of temperature, pressure, etc., are usually not included in the actual simulation software, but are imported from external property libraries in the format of a dynamic link library (DLL). New substances can be introduced by the user, since the creation of additional property-DLLs is possible. The external function libraries are developed and compiled in a C/C++ development environment.

The standard IPSEpro package provided by SimTech already contains a model library for modelling conventional power plant processes (Advanced Power Plant Library). However, this library does not contain any models of gasifiers, driers, gas cleaning equipment, and synthesis reactors. In order to model biomass gasification, fast pyrolysis and fuel synthesis with this library, a large number of models needed to be created. However, for the simulation of biomass gasification and related processes, a special model library called Pyrolysis and Gasification Process Library (PGP_Lib) has been developed by several researchers at the Vienna University of Technology [125, 126] and is licensed by SimTech. The structure of this library has been expanded by Pröll [126] in order to include biomass-related substances (e.g. tars) and to cover inorganic solids (e.g. CaO, K_2O). It also includes models of gasifiers, steam reformers, cyclones, filters, etc. A list of the PGP_Lib models is given in Appendix A. The models contain mass and energy balances and specific equations describing chemical conversions, splitting conditions, empiric correlations from measurements of real gasification plants, etc.

There are four classes of substances in the PGP_Lib [123]:

- Ideal gas mixture (Ar, CH_4, C_2H_4, C_2H_6, C_3H_8, CO, CO_2, H_2, H_2O, H_2S, HCl, N_2, NH_3, HCN, N_2O, NO, O_2, SO_2).
- Water/steam.
- Organic substances (such as biomass, tar and char) that consist of C, H, O, N, S, and Cl, water and ash.
- Inorganic solids, such as dust in gas streams and ash in organic streams.

The simulation of processes, such as fast pyrolysis, Fischer-Tropsch, methanol synthesis and MTG required the introduction of new substances and component models. This is possible on IPSEpro since the software allows the user to edit the source code of a standard model and create new models with the MDK as described above.

5.3 General conditions

In the following sections the ambient conditions and the composition of the feedstock are given. These were kept constant for all process concepts in order to maintain consistency and to make results comparable.

5.3.1 Ambient conditions

Ambient conditions of all process concepts were set to 15°C and 1 atm [5, 41]. Previous modelling work on IPSEpro [41, 126] assumed a relative humidity of 60% which was also used in this study.

5.3.2 Feedstock

For all process concepts throughout this study the same type of biomass is used for consistency. The biomass model is based on wood chips as discussed in section 4.2. The elemental composition of the biomass model is shown in Table 5-2.

In this thesis, plant capacities are expressed in dry tonne per day (dry t/d), where “dry” accounts for 0% water content in the biomass feedstock and 1t is 1000kg. Unless otherwise stated mass yields and energy efficiencies are quoted on a dry ash free (daf) basis where the presence of water and ash in the feedstock are not taken into account for the purposes of the calculation.

Table 5-2: Biomass characteristics [5]

Moisture content	30%
Ash content (wf)	1%
Elemental analysis (wf)	
C	52%
H	6.3%
O	40.32%
N	0.3%
S	0.05%
Cl	0.03%
LHV (dry)	19.7 MJ/kg
LHV (wet)	13.1 MJ/kg

5.4 Biomass preparation

As discussed in section 4.3, biomass drying was done by either an air rotary dryer (fast pyrolysis concept) or a SSD dryer (biomass gasification concepts). The IPSEpro dryer model used in this study was developed by Pröll [126, 127] and is included in the PGP_Lib. It allows modelling of directly heated drying, indirectly heated drying, or combinations of the two. Pröll's dryer model was used for modelling both the SSD dryer and the air rotary dryer.

5.4.1 Superheated steam dryer

The SSD dryer is operated using superheated steam (200^{o}C, 12 bar) [128] which is generated from the downstream synthesis processes. The biomass is dried from 30% to 10% [117]. For all biomass gasification concepts throughout this study the same SSD dryer model was used in order to maintain consistency and to make results comparable.

5.4.2 Air rotary dryer

The air rotary dryer employed for the fast pyrolysis process is operated using air at a temperature of 70°C [5]. The biomass is dried from 30% to 10% water content [5], with the necessary heat being supplied via the mixture of the cooled char flue gas from the pyrolysis reactor and the second fraction of the combusted non-condensable gases (see also section 5.5.5).

5.5 Fast pyrolysis

5.5.1 Modelling approach

As discussed in section 2.4.1.1, fast pyrolysis leads to three products: bio-oil as the main product, gas and char. As discussed in section 5.2.2, the gas streams and char have already been defined on IPSEpro for biomass gasification and can also be adopted for fast pyrolysis. Bio-oil, however, cannot be compared to any of the organic product mixtures from biomass gasification and thus it was necessary to define it in order to model the fast pyrolysis process. In the literature, there is a lot of information on bio-oil's elemental composition which is sufficient for general mass and energy balances since energetic properties such as heating value can be approximated and mass balances can be calculated from the elemental composition of inputs and outputs [5, 126].

The thermodynamic property data of the products were also considered for energy balances calculations as they are necessary for calculating heat transfer, such as the cooling duty for bio-oil condensation. The thermodynamic property data for non-condensable gases and char were described and implemented into IPSEpro by Pröll [126] and were already included in the PGP_Lib. However, thermodynamic data for bio-oil (vapour and liquid phase) is not included in the PGP_Lib and thus it was necessary to introduce and implement such data into the simulation software. For this purpose, a number of representative model substances/compounds contained in the bio-oil were selected to supply thermodynamic data necessary for the calculation of energy balances for the fast pyrolysis process. The selection of representative model substances for bio-oil is not an easy task since the number of chemical species contained in bio-oil is very high, up to 230 substances and more [129, 130]. This is due to the fact that the bio-oil contains a mix of primary and secondary products, which depend on the biomass and the operating conditions of the process [129].

Cottam and Bridgwater [131] followed a similar approach for the thermodynamic modelling of bio-oil. They selected four organic chemical compounds for their study which focused on the techno-economics of fast pyrolysis for fuel production, without giving reasons for their choice except that all four had a molecular weight of approximately 100 g/mol. These substances included: furfural, n-heptane, isovaleric acid, and methyl-isobutyl-ketone. Apart from n-heptane, these compounds are typically found in pyrolysis oils, at least in minor

quantities [132]. Still, none of the main components (e.g. phenols) of either pyrolysis vapours or bio-oil were selected. Therefore, a different set of substances was sought.

Fürnsinn in collaboration with Aston University conducted a comprehensive and thorough research into the selection of representative model substances for the thermodynamic modelling of fast pyrolysis vapours and bio-oil [5]. He first identified the main compounds in fast pyrolysis vapours and bio-oil based on experimental data from the literature. These compounds were further limited to those that are important (in terms of quantity) in both the vapour and the liquid phase of bio-oil and sufficient thermodynamic data is available for each one of them. Table 5-3 shows the five representative model substances of bio-oil proposed by Fürnsinn.

Table 5-3: Bio-oil model substances selected for modelling [5]

Substance class	**Compound**	**wt%**
Organic acids	Acetic acid	18
Aldehydes	Hydroxyacetaldehyde	22
Ketones	Hydroxyacetone	9
Phenols	Guaiacol	46
Alcohols	Methanol	5

These compounds represent the most dominant chemical substance classes found in bio-oil [132, 133], as Fürnsinn intended. The chemical compounds selected by Fürnsinn are in good agreement with results reported by Peacocke [133] who found that the main compounds in the liquid phase are: acetic acid, hydroxyacetaldehyde, hydroxyacetone, phenols and levoglucosan, as well as with the results of Gerdes [134] who, in extensive compound analyses of bio-oil from several types of biomass, equally identified most of the above to be major compounds. In addition, Evans and Milne [129] conducted a comprehensive study of the formation of fast pyrolysis vapours and their chemical composition. They identified the major products of fast pyrolysis of wood by means of molecular-beam mass spectrometric sampling at real time. They reported approximately 40 compounds that were detected in mass spectroscopy of fast pyrolysis vapours, although some of them were of relative abundance. These also included the substances selected by Fürnsinn. Therefore, Fürnsinn's set of representative model substances for the thermodynamic modelling of pyrolysis vapours and bio-oil was selected for this study.

5.5.2 Thermodynamic modelling

As discussed in the previous section, the elemental composition of bio-oil is not fully sufficient for calculating energy balances for the fast pyrolysis process. From this, only the lower and higher heating value of bio-oil can be estimated via the method of Boie which is used in IPSEpro for the calculation of LHVs of solid and liquid organic fuels [127]. Therefore, as discussed in the previous section, five model substances contained in the bio-oil were selected to supply additional thermodynamic data necessary for the calculation of energy balances. In the following, the methodology for the calculation of thermodynamic state variables for both the vapour and the liquid phase of bio-oil is described.

5.5.2.1 Vapour phase

The enthalpy of a compound can be calculated from the enthalpy of formation and the heat capacity as follows:

$$\mathrm{H(T)} = \Delta \mathrm{h}^{0}_{\mathrm{f},298} + \int_{298.15}^{\mathrm{T}} \mathrm{C_p(T)} \cdot \mathrm{dT} \qquad (5\text{-}1)$$

Therefore, in order to calculate the enthalpy of each model substance in the vapour phase, the enthalpy of formation and the heat capacity must be known.

Enthalpy of formation

The Joback method was used to estimate the enthalpy of formation for each model substance. The Joback method is a widely used group contribution method which estimates the thermodynamic properties of chemical compounds from their molecular structure [5, 135]. With this method, thermodynamic properties of a chemical compound (e.g. methanol) are calculated based on characteristic groups of atoms (e.g. -OH) found in the compound. The enthalpy of formation for each model substance in the vapour phase of bio-oil was calculated from the following equation [135]:

$$\Delta \mathrm{h}^{0}_{\mathrm{f},298} = 68.29 + \sum \Delta H_{f,i} \cdot N_i \qquad (5\text{-}2)$$

where N_i represents the number of each characteristic group in the model substance (e.g. one methyl group -CH_3 in methanol). The $\Delta H_{f,i}$ is the contribution of each characteristic group in the enthalpy of formation of the model substance and its value for each group can

be found in Perry's Chemical Engineers' Handbook [135]. The calculation of the enthalpy of formation for each model substance is shown in Table 5-4.

Heat capacity

The Joback method was also used for the calculation of heat capacities of the selected model substances. With this method, heat capacities are calculated as a function of temperature. To this end, a polynomial equation is proposed by Joback [135]:

$$C_p(T) = A + B \cdot T + C \cdot T^2 + D \cdot T^3 \qquad (5\text{-}3)$$

The polynomial coefficients A, B, C, D are valid from 273 K to 1000 K and are calculated from the following equations [135]:

$$A = \sum N_i \cdot a_i - 37.93 \qquad (5\text{-}4)$$

$$B = \sum N_i \cdot b_i + 0.210 \qquad (5\text{-}5)$$

$$C = \sum N_i \cdot c_i - 3.91 \cdot 10^{-4} \qquad (5\text{-}6)$$

$$D = \sum N_i \cdot d_i + 2.06 \cdot 10^{-7} \qquad (5\text{-}7)$$

where a_i, b_i, c_i, and d_i are the characteristic group contributions to the polynomial coefficients A, B, C and D, respectively.

Table 5-4 shows the group contributions a_i, b_i, c_i, and d_i which were found in Perry's Chemical Engineers' Handbook [135]. The same table shows the calculation of the polynomial coefficients A, B, C and D for each of the five model substances specified in section 5.5.1.

Table 5-4: Calculation of enthalpies of formation for the selected bio-oil model substances in the vapour phase

Hydroxyacetone						
Groups	N_i	ΔH_f kJ/mol	a J/mol·K	b J/mol·K	c J/mol·K	d J/mol·K
CH_3	1	-76.45	1.95E+1	-8.08E-3	1.53E-4	-9.67E-8
CH_2	1	-20.64	-9.09E-1	9.50E-2	-5.44E-5	1.19E-8
CO	1	-133.22	6.45	6.70E-2	-3.57E-5	2.86E-9
OH	1	-208.04	2.57E+1	-6.91E-2	1.77E-4	-9.88E-8
		$\sum \Delta H_i \cdot N_i$ -438.35	$\sum N_i \cdot a_i$ 5.07E+1	$\sum N_i \cdot b_i$ 8.48E-2	$\sum N_i \cdot c_i$ 2.40E-4	$\sum N_i \cdot d_i$ -1.81E-7
		$\Delta h^0_{f,298}$ -370.06	A 1.28E+1	B 2.95E-1	C -1.51E-4	D 3.87E-7

Methanol						
Groups	N_i	ΔH_f kJ/mol	a J/mol·K	b J/mol·K	c J/mol·K	d J/mol·K
CH_3	1	-76.45	1.95E+1	-8.08E-3	1.53E-4	-9.67E-8
OH (alcohol)	1	-208.04	2.57E+1	-6.91E-2	1.77E-4	-9.88E-8
		$\sum \Delta H_i \cdot N_i$ -284.49	$\sum N_i \cdot a_i$ 4.52E+1	$\sum N_i \cdot b_i$ -7.72E-2	$\sum N_i \cdot c_i$ 3.30E-4	$\sum N_i \cdot d_i$ -1.96E-7
		$\Delta h^0_{f,298}$ -216.20	A 7.27	B 1.33E-01	C -6.10E-05	D 1.0E-08

Guaiacol						
Groups	N_i	ΔH_f kJ/mol	a J/mol·K	b J/mol·K	c J/mol·K	d J/mol·K
CH_3	1	-76.45	1.95E+1	-8.08E-3	1.53E-4	-9.67E-8
=C< (ring)	2	46.43	-8.25	1.01E-1	-1.42E-4	6.78E-8
=CH- (ring)	4	2.09	-2.14	5.74E-2	-1.64E-6	-1.59E-8
OH (phenol)	1	-221.65	-2.81	1.11E-1	-1.16E-4	4.94E-8
-O-	1	-132.22	2.55E+1	-6.32E-2	1.11E-4	-5.48E-8
		$\sum \Delta H_i \cdot N_i$ -329.1	$\sum N_i \cdot a_i$ 1.73E+1	$\sum N_i \cdot b_i$ 4.71E-1	$\sum N_i \cdot c_i$ -1.43E-4	$\sum N_i \cdot d_i$ -3.01E-8
		$\Delta h^0_{f,298}$ -260.81	A -2.08E+1	B 6.81E-1	C -5.34E-4	D 1.76E-7

Acetic acid						
Groups	N_i	ΔH_f kJ/mol	a J/mol·K	b J/mol·K	c J/mol·K	d J/mol·K
CH_3	1	-76.45	1.95E+1	-8.08E-3	1.53E-4	-9.67E-8
COOH	1	-426.72	2.41E+1	4.27E-2	8.04E-5	-6.87E-8
		$\sum \Delta H_i \cdot N_i$ -503.17	$\sum N_i \cdot a_i$ 4.36E+1	$\sum N_i \cdot b_i$ 3.46E-2	$\sum N_i \cdot c_i$ 2.33E-4	$\sum N_i \cdot d_i$ -1.65E-7
		$\Delta h^0_{f,298}$ -434.88	A 5.67	B 2.45E-1	C -1.58E-4	D 4.06E-8

Hydroxyacetaldehyde						
Groups	N_i	ΔH_f kJ/mol	a J/mol·K	b J/mol·K	c J/mol·K	d J/mol·K
CH_2	1	-20.64	-9.09E-1	9.50E-2	-5.44E-5	1.19E-8
CHO	1	-162.03	3.09E+1	-3.36E-2	1.60E-4	-9.88E-8
OH	1	-208.04	2.57E+1	-6.91E-2	1.77E-4	-9.88E-8
		$\sum \Delta H_i \cdot N_i$ -390.71	$\sum N_i \cdot a_i$ 5.57E+1	$\sum N_i \cdot b_i$ -7.70E-3	$\sum N_i \cdot c_i$ 2.83E-4	$\sum N_i \cdot d_i$ -1.86E-7
		$\Delta h^0_{f,298}$ -322.42	A 1.77E+1	B 2.02E-1	C -1.08E-4	D 2.03E-8

Enthalpy of bio-oil in vapour phase

The next step was to combine equation 5.3, which was used for the calculation of heat capacities, with equation 5.1 in order to calculate the enthalpy for each model substance. The resulting equation is given below:

$$\mathrm{H_i(T)} = \Delta h^0_{f,298} + \int_{298.15}^{T} \mathrm{C_p(T)}\cdot \mathrm{dT} = \Delta h^0_{f,298} + \int_{298.15}^{T} (A + B\cdot T + C\cdot T^2 + D\cdot T^3)\cdot \mathrm{dT}$$

$$= \Delta h^0_{f,298} + \left[A\cdot T + \frac{1}{2}B\cdot T^2 + \frac{1}{3}C\cdot T^3 + \frac{1}{4}D\cdot T^4\right]_{298.15}^{T} \qquad (5.8)$$

Finally, the enthalpy of bio-oil in the vapour phase was estimated in IPSEpro using the following equation which is the weighted average of the enthalpies of the model substances:

$$\mathrm{H(T)} = \sum H_i(T)\cdot x_i \qquad (5.9)$$

where $\mathrm{H_i(T)}$ is the enthalpy of each model compound as a function of temperature (equation 5.8) and x_i is the mass fraction of each model substance as given in Table 5-3 (see section 5.5.1).

5.5.2.2 Liquid phase

For the fast pyrolysis liquids, the heat capacity for each model substance was estimated by using another group contribution method, the Chueh and Swanson method [135]. This method provides an estimate of heat capacities at 293 K. Since bio-oil appears at room temperature (20°C) in the fast pyrolysis model, heat capacities at 293 K can reasonably be used. For each characteristic group a certain value for the heat capacity can be found in tables and the heat capacity of the molecule results from the addition of all group values:

$$C_p = \sum C_{p,i}\cdot N_i \qquad (5\text{-}10)$$

Table 5.5 shows the characteristic group contributions $C_{p,i}$ [135] and the calculation of the heat capacity for each model substance. The same table shows the enthalpy of formation values for each model substance in the liquid phase [136, 137].

Table 5-5: Thermodynamic properties of the selected model substances in the liquid phase. Literature values: [1] [137], [2] [136]

Hydroxyacetone		
Groups	N_i	$C_{p,i}$ J/mol·K
CH_3	1	36.82
CH_2	1	30.38
CO	1	52.97
OH	1	44.77
C_p	164.94 J/mol·K	
$\Delta h^0_{f,298}$ [2]	-410.8 kJ/mol	

Methanol		
Groups	N_i	$C_{p,i}$ J/mol·K
CH_3	1	36.82
OH	1	44.77
C_p	81.59 J/mol·K	
$\Delta h^0_{f,298}$ [1]	-238.6 kJ/mol	

Guaiacol		
Groups	N_i	$C_{p,i}$ J/mol·K
CH_3	1	36.82
=C<	2	12.13
=CH-	4	22.18
OH	1	44.77
-O-	1	35.15
C_p	229.72 J/mol·K	
$\Delta h^0_{f,298}$ [2]	-287.4 kJ/mol	

Acetic acid		
Groups	N_i	$C_{p,i}$ J/mol·K
CH_3	1	36.82
COOH	1	79.91
C_p	116.73 J/mol·K	
$\Delta h^0_{f,298}$ [1]	-484.1 kJ/mol	

Hydroxyacetaldehyde		
Groups	N_i	$C_{p,i}$ J/mol·K
CH_2	1	30.38
CHO	1	52.97
OH	1	44.77
C_p	128.12 J/mol·K	
$\Delta h^0_{f,298}$ [2]	-357.2 kJ/mol	

Heat capacities of liquids are much less dependent on temperature than gases [5, 126] and since bio-oil appears at a low temperature (40°C) in the fast pyrolysis model, no temperature dependence of the liquid heat capacities was modelled. Thus, the enthalpy of each model substance in the liquid phase was estimated by the following equation:

$$H_i(T) = \Delta h^0_{f,298} + \int_{298.15}^{T} C_p(T) \cdot dT = \Delta h^0_{f,298} + C_p(T - 298.15) \qquad (5\text{-}11)$$

where C_p is the heat capacity of each model substance calculated from equation 5-10. As with the vapour phase, the enthalpy of bio-oil in the liquid phase was also estimated as the weighted average of the enthalpies of the model substances.

5.5.3 Fast pyrolysis reactor

5.5.3.1 Model structure

As with gasification, where the IPSEpro gasifier model only consists of a black-box approach with only few major chemical reaction relationships, fast pyrolysis modelling equally needs to be cast in simplicity in order to allow for efficient integration into IPSEpro. Thus, while inclusion of chemical kinetics or complex thermodynamic relationships are beneficial for the understanding of what takes place inside the reactor, in this study the fast pyrolysis reactor model was built to describe the mere relation between biomass and fast pyrolysis products.

The IPSEpro model of the fast pyrolysis reactor is shown in Figure 5.2. The reactor was a fluidised bed system for the reasons already discussed in section 4.4. In fluidised bed reactors, some heat is supplied via the fluidisation gas but heat requirements cannot be met by the fluidisation gas alone. Therefore additional heating via the reactor walls or heating coils was also employed. As with all PGP_LIb models a gaseous heat carrier was assumed for the indirect heat transfer. A description of the input and output streams of the fast pyrolysis reactor is given in Table 5-6.

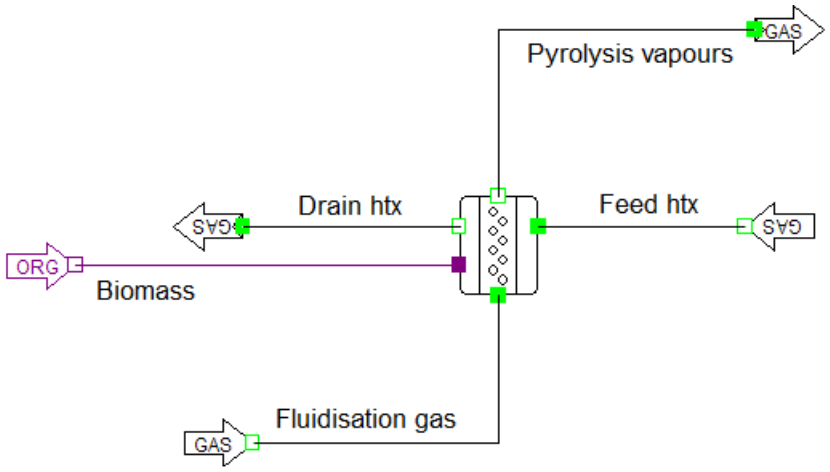

Figure 5-2: IPSEpro model of the fast pyrolysis reactor

Table 5-6: Input and output streams of the fast pyrolysis reactor model

Input streams	**Characterisation**
Biomass	Elemental composition, water and ash content, enthalpy as a function of temperature (Pröll [126])
Fluidisation gas	Gas composition (described in section 5.2.2)
Feed indirect heating	Gas composition

Output streams	**Characterisation**
Pyrolysis vapours	• Fast pyrolysis vapours Elemental composition, enthalpy as a function of temperature based on model substances (section 5.5.2) • Other gases Gas composition (section 5.2.2) • Char Elemental composition, enthalpy as a function of temperature based on model substances (Pröll [126]) • Dust Elemental composition, enthalpy as a function of temperature based on model substances (Pröll [126])
Drain indirect heating	Gas composition (same as feed indirect heating)

5.5.3.2 Mass balances

As with the biomass gasifier IPSEpro model, the fast pyrolysis reactor model employs elemental mass balances of all components entering and leaving the reactor in order to estimate the relative amount of products formed. Similar to other IPSEpro models of the PGP_Lib (e.g. biomass gasifier), the elemental mass balances were set up for carbon (C), hydrogen (H), oxygen (O), nitrogen (N), argon (Ar), sulphur (S) and chlorine(Cl).

The three product classes (see Table 5-6 in section 5.5.3.1) were determined in both total mass and composition:

- Fast pyrolysis vapours (total amount produced and elemental composition)
- Char (total amount produced and elemental composition)
- Dust from biomass ash which is carried into the reactor via the fluidisation gas (total amount, elemental composition)

The total amount of gases produced resulted from the elemental mass balances. However, some gas compounds had to be specified in order to get a fully determined equation system for the fast pyrolysis reactor model. The following section describes the approach followed to estimate the amount of products formed from fast pyrolysis.

Fast pyrolysis vapours and char

As described in section 2.4.1, the amount of vapours and thus bio-oil produced, as well as the quantity of char formed in the fast pyrolysis process highly depend on the reaction conditions. Cottam and Bridgwater [131], whose work was mentioned in section 5.5.1, estimated the yields of dry bio-oil (i.e. vapours), char, gases and water as a function of temperature based on experimental results from wood. The equations for estimating the mass yields of fast pyrolysis vapours and char by Cottam and Bridgwater [131], were also adopted in this study and are as follows:

$$y_{bio-oil}(T) = -402.91 + 1.86 \cdot T - 0.00184 \cdot T^2 \qquad (5.12)$$

$$y_{char}(T) = 521.2 \cdot 10^{(-0.00312 \cdot T)} \qquad (5.13)$$

The above empirical relationships for estimating the mass yields of dry bio-oil and char were based on a dry ash-free (daf) wood feedstock. The amounts of water and other gases produced were calculated in IPSEpro via elemental mass balances.

For the elemental composition of bio-oil and char produced in the process, values given from Fürnsinn were used [5]. These values were based on experimental studies from the literature. Table 5-7 shows the elemental composition of bio-oil used in this study.

Table 5-7: Bio-oil elemental composition (wt%, dry basis); literature values and model settings

	Woody biomass [5]	**Model**
Temperature	500 ^{o}C	500 ^{o}C
C	55 %	55 %
H	6.6 %	6.5 %
O	38.5 %	38.5 %
N	0.1 %	-
S	0.05 %	-
Cl	0.03 %	-

According to Fivga [132], the nitrogen content of bio-oil from woody biomass is very low (0-0.02%), thus the nitrogen content of bio-oil was set to zero in the model. Due to the lack of data in the literature for the sulphur and chlorine content of bio-oil, Fürnsinn assumed that they were 0.05 % and 0.03 % respectively. These values were based on the simple assumption that both are slightly lower than nitrogen, but in the range of the corresponding values for wood biomass. It should be noted that the sum of Fürnsinn's model values is not 100% as it should be and Fürnsinn does not give any explanation on that. According to Bridgwater [17, 22] and Fivga [132], the sulphur and chlorine content of bio-oil from woody biomass are extremely low (<0.01%) and thus they were both set to zero.

Table 5-8 shows the elemental composition of char used in this study. Again, as opposed to Fürnsinn's model the sulphur and chlorine content were set to zero for the reasons described above. The selected composition is in accordance to Stahl et al. [138] who do not provide any values for the sulphur and chlorine content of fast pyrolysis char. Thus, they were both assumed to be very low to significantly affect the overall mass balances of the process.

Table 5-8: Char elemental composition (wt%, dry basis) for fast pyrolysis; literature values and model settings.

	Woody biomass [5]	**Model**
Temperature	500°C	500°C
C	90-92 %	89.7 %
H	3 %	3 %
O	4-6 %	6.8%
N	0.4 %	0.4 %
S	0.05 %	-
Cl	0.03 %	-

Other gases

For the gas compounds of the fast pyrolysis process (e.g. CO, CO_2), Fürnsinn used literature values for the yields of the major gas compounds based on the dry ash-free biomass input. These values were also adopted in this study and are shown in Table 5-9.

Table 5-9: Fast pyrolysis gas yields [5]. Process temperature: 500°C

	% yield	wt% (dry gas)
H_2	0.02	0.2
CO	4.22	43.4
CO_2	4.72	48.5
CH_4	0.39	4.0
C_2H_4	0.17	1.8
C_2H_6	0.04	0.4
C_3H_8	0.16	1.6

The values for CO, H_2, CH_4, C_2H_4, C_2H_6 and C_3H_8 were set in IPSEpro to the values shown in Table 5-9. It was also assumed that neither oxygen, nitrogen nor NO were formed or consumed during the fast pyrolysis reactions. The amounts of sulphur and the remaining nitrogen containing gases were calculated from the respective elemental balances.

5.5.3.3 Energy balance

As with all IPSEpro unit models, the energy balance (i.e. enthalpy balance) of the fast pyrolysis reactor is given by the following equation:

$$\sum \dot{h}\,(in) = \sum \dot{h}\,(out) \qquad (5-14)$$

For the fast pyrolysis reactor model the above equation was formulated as following:

$$\dot{h}(biomass) + \dot{h}(fluid.gas) + \dot{h}(htx,in) = \dot{h}(pyrol.vapours) + \dot{h}(htx,out) + Q_{loss} \cdot 3600 \qquad (5-15)$$

where Q_{loss} is the heat loss from the reactor in kW and $\dot{h}$ is the enthalpy flow in kJ/h defined as:

$$\dot{h} = \dot{m} \cdot h^{*} \qquad (5-16)$$

where $\dot{m}$ is the massflow of the stream in kg/h and h^{*} is the enthalpy of the stream in kJ/kg.

From equation 5-15 the amount of heat required for the pyrolysis reactions is defined as:

$$Q_{htx} = \left[\dot{h}(htx,in) - \dot{h}(htx,out)\right]/3600 \qquad (5-17)$$

5.5.3.4 Reactor model variables

Apart from the mass and energy balances equations, some variables were required to describe the model. These variables are shown in Table 5-10. Variables represent numerical data of an IPSEpro model and can either be prescribed by the user or calculated while the system is solved on IPSEpro.

Table 5-10: Variables of the fast pyrolysis reactor model

Variable	Unit	Description
dp_gas	bar	Pressure drop of the fluidisation gas; also determines the pressure of vapours and other gases.
dp_htx	bar	Pressure drop of the indirect heating stream
Q_htx	kW	Power of indirect heating
Q_loss	kW	Heat loss from the reactor
ratio_fluid_biomass	kg/kg	Mass flow of fluidisation gas to biomass input ratio

5.5.4 Condensation unit model

After fast pyrolysis, the resulting gases pass through a set of cyclones where dust and char are extracted. IPSEpro models of particulates removal units, such as filters and cyclones, have already been developed by Pröll [126] and are included in the PGP_Lib. After removal of dust and char, the gases enter a condensation unit where they are cooled

and condensed into bio-oil. The condensation unit model was not available in the PGP_Lib and thus it was built specifically for this study.

5.5.4.1 Model structure

The condensation unit model is shown in Figure 5.3. Some simplifications listed below were made in order to build an easy-to-operate model that could be efficiently integrated into IPSEpro:

- Black box model; no kinetics or construction details of the unit.
- Same elemental composition for fast pyrolysis vapours and bio-oil.
- Model substances for fast pyrolysis vapours and bio-oil were the same, only in different physical state. Therefore, no chemical reactions occurred during condensation.
- Simple indirect heat exchange (cooling water) for bio-oil condensation.

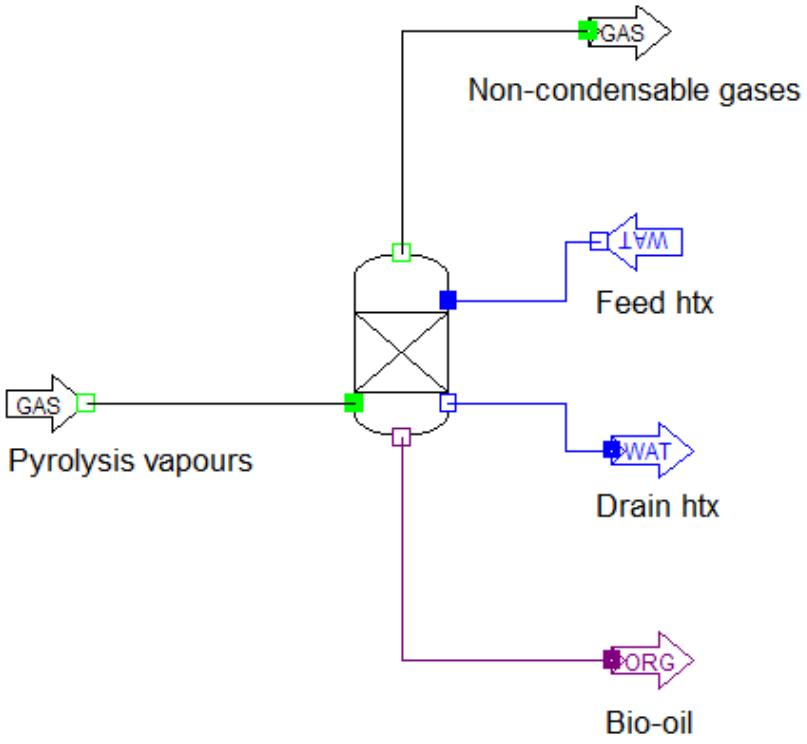

Figure 5-3: IPSEpro model of the bio-oil condensation unit

In fact, chemical reactions, such as oligomerisation, do take place during condensation [129]. However, the contribution of the enthalpy of reaction to the overall energy balance was considered insignificant due to the large amount of heat transferred to the cooling medium since the gases are cooled down by 460^{o}C. Furthermore, the enthalpy of reaction influences only the cooling duty of the condensation unit which it is not included in the calculation of the overall energy efficiency of the process (see section 5.12.1).

The chemical reactions that take place during condensation change the chemical structure of the vapours compounds but not their elemental composition [5]. Since the chemical properties of bio-oil are not of interest in this study but only its heating value based on elemental composition, the assumption of equal elemental composition of vapours and bio-oil is justified.

Condensation via simple indirect heat exchange with cooling water was assumed. However, this condensation method can cause preferential deposition of lignin-derived components leading to liquid fractionation and eventually blockage in pipelines and heat exchangers [17]. Thus, quenching with previously made bio-oil (e.g. Dynamotive, Ensyn) or a hydrocarbon solvent is usually employed. For the reasons highlighted above, neither the cooling duty nor the nature of the cooling medium of the pyrolysis condenser are of interest in the process performance assessment, thus a simple condensation model was built.

5.5.4.2 Mass and energy balances

The condenser was modelled without any change of chemical composition of the participating phases (see also previous section), thus no chemical species were consumed or formed. The mass balance equations of this model were component specific and forced equal amounts and compositions at feed and drain of each stream.

The energy balance equation was similar to that of the fast pyrolysis reactor:

$$\dot{h}(pyrol.vapours) = \dot{h}(bio-oil) + \dot{h}(cond.gases) + Q_{clg} \cdot 3600 + Q_{loss} \cdot 3600 \qquad (5-18)$$

where Q_{clg} is the cooling duty (kW) of the condenser estimated from the following equation:

$$Q_{clg} = \left[\dot{h}(clg,out) - \dot{h}(clg,in)\right]/3600 \qquad (5-19)$$

5.5.4.3 Condensation unit model variables

Several variables were required to describe the condensation unit model. These are briefly described in Table 5-11.

Table 5-11: Variables of the condensation unit model

Variable	Unit	Description
dp_gas	bar	Pressure difference between pyrolysis vapours and non-condensable gases
dp_org_gas	bar	Pressure difference between exiting gas and bio-oil
dp_clg	bar	Pressure drop of the cooling stream
dt_gas	^{o}C	Temperature difference between pyrolysis vapours and non-condensable gases
dt_org_gas	^{o}C	Temperature difference between pyrolysis vapours and bio-oil
sep_eff_vap	%	Separation efficiency of pyrolysis vapours
rho_drain_org	kg/m^3	Density of bio-oil. Set to 1200 kg/m^3 [139].
Q_clg	kW	Cooling duty of the water heat exchanger
Q_loss	kW	Heat loss from the reactor

5.5.5 Fast pyrolysis process concept - Overall model

The flow sheet of the fast pyrolysis process concept is shown in Figure 5-4. Biomass (wood chips) was dried from 30% to 10% water content using an air rotary dryer (see sections 4.3 and 5.4.2). The dried biomass was then fed to the fast pyrolysis reactor, where the product mix was obtained at 500^{o}C [17]. The char and ash were separated in a set of cyclones, after which the pyrolysis vapours were condensed to bio-oil.

As already discussed in section 4.4, the heat demand of the fast pyrolysis reactor was met by the combustion of the non-condensable gases and part of the char. The cooled non-condensable gases were combusted with little oxygen surplus (λ = 1.05) to avoid high oxygen concentration in the combustor flue gas, since part of the latter was used as fluidisation medium for the fast pyrolysis reactor [5]. A flue gas temperature of about 520^{o}C was achieved which could thus be directly fed into the reactor.

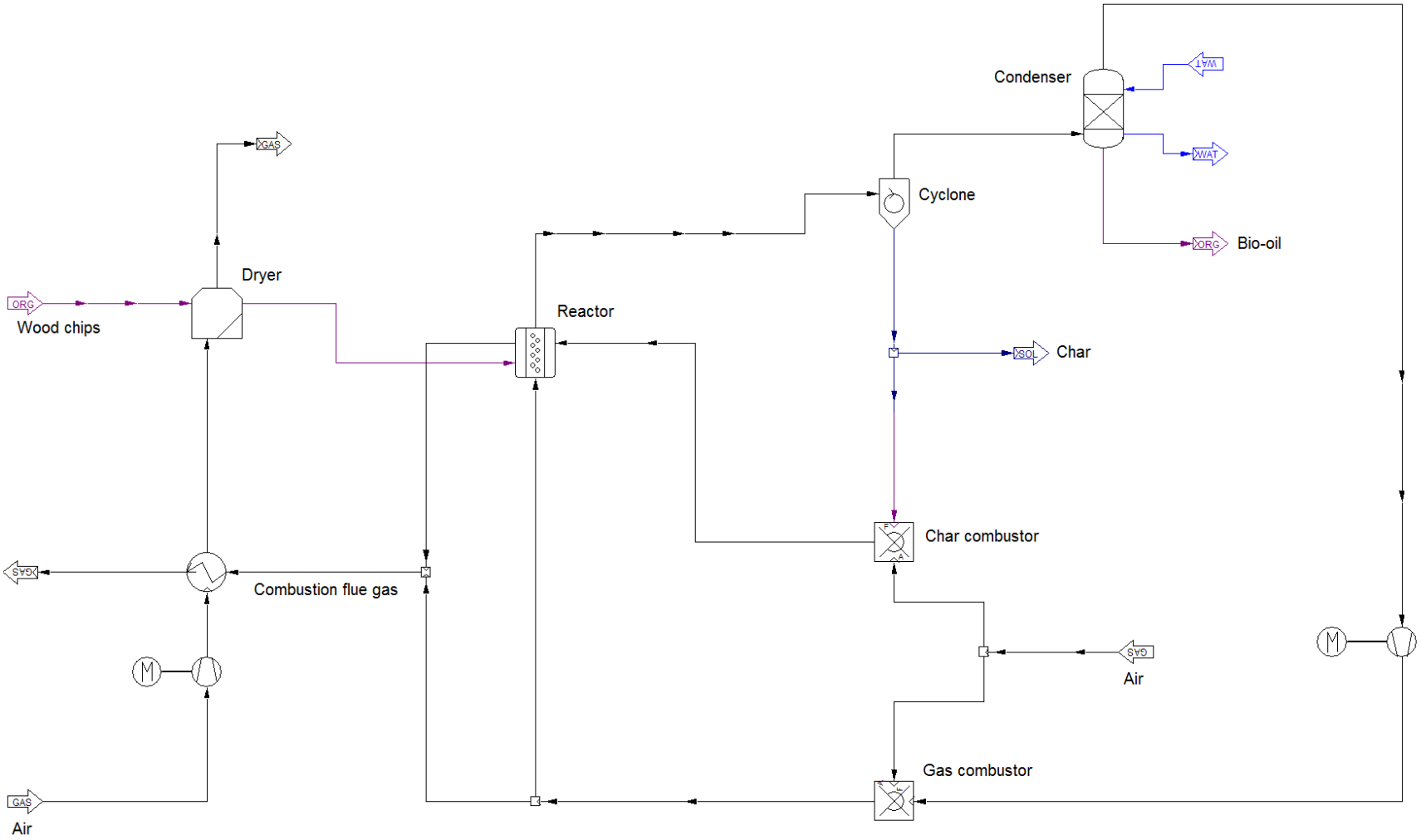

Figure 5-4: Flow sheet of the fast pyrolysis process

The char was combusted to supply the extra heat needed for the fast pyrolysis process. The temperature of the flue gas stream from the char combustor was set to 700°C [5]. The flue gas stream of the char combustor exited the fast pyrolysis reactor at 510°C [5]. It was then combined with flue gas from the gas combustor and passed through a heat exchanger to supply heat to the air dryer.

5.5.5.1 Results

The results of the simulation analysis of the fast pyrolysis process are summarised in Table 5-12. In this study, the energy efficiency of the fast pyrolysis concept is defined as the ratio between the total energy in bio-oil (organics only) and that in the biomass feedstock (daf basis):

$$\eta_{pyrolysis} = \frac{\dot{M}_{bio-oil} \cdot LHV_{bio-oil}}{\dot{M}_{biomass} \cdot LHV_{biomass}} \qquad (5-20)$$

where $\dot{M}_{bio-oil}$ is the mass flow (kg/h) of bio-oil, $LHV_{bio-oil}$ is the lower heating value (kJ/kg) of bio-oil, $\dot{M}_{biomass}$ is the mass flow input (kg/h) of the daf biomass and $LHV_{biomass}$ is the lower heating value (kJ/kg) of the daf biomass feed.

It should be noted that almost all the pyrolysis char (about 98%) needed to be combusted to meet the heat requirements of the fast pyrolysis reactor. This was due to the low heating value of the non-condensable gases since the pyrolysis gases were diluted with combustion flue gas used as fluidisation medium for the reactor.

The results from the simulation of the fast pyrolysis process with IPSEpro are consistent with those from recent modelling studies on fast pyrolysis [5, 105]. Furnsinn [5] reports a mass yield of 66% and a plant energy efficiency of 70%, whereas Rogers [105] reports mass yields in the range of 50 - 74% and energy efficiencies in the range of 55 - 70%.

Table 5-12: Settings and results of the fast pyrolysis process simulation

Biomass		
LHV wet biomass	kJ/kg	13,056
Water content	%	30
Ash content	%	1
Mass flow (wet)	kg/h	23,810
LHV daf biomass	kJ/kg	19,897
Mass flow (dry)	kg/h	16,667
Mass flow (dry)	t/d	400
Bio-oil		
LHV (organic fraction)	kJ/kg	21,103
HHV (organic fraction)	kJ/kg	22,522
LHV (as produced)	kJ/kg	14,582
HHV (as produced)	kJ/kg	16,284
Water content	%	27
Mass flow (as produced)	kg/h	15,004
Mass flow (as produced)	t/d	360.1
Char		
Mass flow (prior to combustion)	kg/h	2,519
Mass flow (after combustion)	kg/h	49.4
Mass flow (after combustion)	t/d	1.185
Energy efficiency (eqn. 5-20)	%	69.7
Bio-oil mass yield (daf basis)	%	65.8

It is also worthwhile comparing the results of the model with the reported mass yields of Dynamotive's fast pyrolysis pilot plant [140]. Table 5-13 shows the results of the model in comparison with those from Dynamotive's plant. The model was rerun with a biomass water content of 3% and ash content of 1.5% to make results comparable.

Table 5-13: Comparison of the fast pyrolysis model with Dynamotive's pilot plant [140]

	Dynamotive	Model
Settings		
Biomass type	wood	wood
Biomass water content	3%*	3%
Biomass ash content	1.5%*	1.5%
Results		
Bio-oil water content	22.5%*	21%
Bio-oil LHV	16.5 MJ/kg*	16.2 MJ/kg
Mass yield	70%	66%

*The value used is the average of the values reported in the reference

Table 5-13 shows that the fast pyrolysis simulation results of this study which were based on reported experimental data are consistent with reported data from an industrial pilot plant.

5.6 Gasification

5.6.1 General gasifier model

As discussed in section 4.5, gasification of biomass was done using either a circulating fluidised bed (CFB concepts) or an entrained flow gasifier (EF concepts). The IPSEpro gasifier model used in this study was developed by Pröll [126] and is included in the PGP_Lib. Pröll's gasifier model is a general balance model of a biomass gasifier which consists of elemental mass balances, energy balances and some chemical equilibrium relationships. As with the fast pyrolysis reactor model (see section 5.5.3), since chemical reactions take place during gasification, the mass balances of the gasifier model are formulated on the basis of chemical elements. This is the approach followed for all IPSEpro models that include chemical reactions since production or consumption of chemical species can occur in these models. Only inorganic solids (char, ash) are treated as inert, i.e. the conservation of chemical species is formulated for the solids [127]. For char and tar composition, the model relies on prescribed values determined by measurements [127].

For the product gas composition, the elemental mass balances determine the concentrations of Ar, H_2S and HCl. The equilibrium of the CO shift reaction can be set by the user (a value of zero defines equilibrium) in order to determine the CO/CO_2 ratio in the product gas. The hydrogen balance calculates the amount of H_2 in the product gas, the oxygen balance yields H_2O and the nitrogen balance N_2. Finally, the compositions of all the other components (C_2H_4, C_2H_6, C_3H_8, CH_4, NH_3, HCN) are set by the user.

Proll's model was used for modelling both the CFB and the entrained flow gasifier, however operating conditions, syngas composition and gasification medium requirements were different for the two gasifiers. This is further discussed in the following two sections.

5.6.2 Circulating Fluidised Bed gasifier

Biomass dried to 10% moisture using an SSD dryer (see section 5.4.1) is fed to a pressurised CFB gasifier. As discussed in section 4.5, the dried fuel was pressurised in a lock hopper system and was fed into the pressurised gasifiers via a pressurised vessel [112]. IPSEpro includes a model which increases the pressure of an organic stream and simulates a lock hopper. This model was used to pressurise the dried biomass stream before it passes to the gasifiers. As discussed in section 4.5, a lock hopper system requires large amounts of inert gas, usually N_2, in order to pressurise the dried fuel which results in lower gasification efficiencies due to the dilution of the product gas. CO_2 produced from the Rectisol unit was used instead of N_2 as inert gas for the lock hopper system. Higman et al. [141] report inert gas requirements of 0.09 kg/kg dry biomass for pressurised gasifiers (~25 bar). This results in a 180 t/d CO_2 requirement for the lock hopper system of both gasifiers.

Oxygen at 95% purity and steam are fed into the gasifier which operates at 28 bar and 870^{o}C [91]. For both CFB and EF gasifiers, the amount of oxygen entering the gasifier was not set, as it was defined by the temperature of the gasifier. The amount of steam was adjusted accordingly in order to have a syngas composition similar to reported experimental results [36, 142, 143]

5.6.3 Entrained Flow Gasifier

The entrained flow gasifier operates at 1400^{o}C and 28 bar [91]. As discussed in section 4.5, the high temperature of the entrained flow gasifier results in a methane and tar-free

product gas [110, 144]. However, in order to reach this high temperature the EF gasifier requires higher amounts of oxygen than the CFB gasifier. Table 5-14 shows the syngas composition for both gasifiers. More hydrogen and carbon monoxide are formed from the entrained flow gasifier as a result of the water-gas-shift reaction (see section 2.7.2) and the reforming of light hydrocarbons (see section 2.7.2). In general, according to Le Chatelier's principle, higher temperatures favour the reactants in exothermic reactions (e.g. Water-gas-shift reaction) and favour the products in endothermic reactions (e.g. steam reforming reaction). The CFB gasifier, on the other hand, produces tar and a significant amount of methane and other light hydrocarbons, thus requiring downstream reforming. This is discussed in the following section.

Table 5-14: Characteristics and raw syngas composition (vol %) for the gasification concepts evaluated in this study

	CFB gasifier	EF gasifier
P (bar)	28	28
T (^{o}C)	850	1400
Oxygen (kg/kg dry feed)	0.32	0.6
Steam (kg/kg dry feed)	0.17	0.15
Gas composition (vol% wet basis [dry basis])		
H_2O	12.6 [0]	25 [0]
H_2	28.3 [32.4]	25.9 [34.5]
CO	26 [29.8]	37.1 [49.5]
CO_2	21.2 [24.2]	10.8 [14.4]
CH_4	10.5 [12]	0 [0]
C_{2+}	0.52 [0.6]	0 [0]
Ar	0.27 [0.3]	0.42 [0.55]
N_2	0.56 [0.62]	0.75 [0.99]
NH_3	0.005 [5.8 x10^{-3}]	0 [0]
H_2S	0.02 [0.024]	0.017 [0.023]
HCl	0.01 [0.013]	0.009 [0.013]
HCN	5 x10^{-4} [6 x10^{-4}]	0 [0]

5.7 Gas cleaning & conditioning - CFB gasifier

The gas cleaning section for the CFB gasifier is shown in Figure 5-11 in section 5.12.2.2. After the initial particulates (char and ash) separation by a cyclone, the syngas passes to the tar cracker where tars are destroyed at 875^{o}C by addition of oxygen and steam (see

also section 4.6). It is assumed that light hydrocarbons (C_1-C_3) are converted at 99% conversion to syngas [117-120]. Tars are assumed to be fully converted into gaseous compounds [114] and all gases are determined in the model via elemental mass balances. The tar cracker/reformer model used in this study was developed by Pröll [126] and is included in the PGP_Lib. Proll's model is a general steam reformer model (i.e. indirectly heated) which can also be used as a water-gas-shift reactor. The original model was modified to include the molar steam to carbon ratio (S/C) to be specified in order to have an autothermal reformer model. This is because steam reformers are more suitable for hydrogen production applications due to their high H_2/CO ratio (~3). Furthermore, an autothermal reformer holds the advantage of relatively simple design compared to a steam reformer due to the absence of heat transfer hardware which also results in higher thermal efficiency [145]. The S/C ratio of the autothermal tar cracker/reformer model was set at 2 for higher conversion of light hydrocarbons as proposed by Zeman and Hofbauer [146].

The tar free syngas is then cooled to 280^{o}C by a heat exchanger yielding steam which is used by the tar cracker. The cooled syngas passes through a bag filter [36] where the remaining particulates are removed. The gas cleaning section for the CFB gasifier is shown in Figure 5-11 in section 5.12.2.2.

After the final particulate removal the syngas is fed to the Rectisol unit where CO_2 and sulphur compounds are removed (see also section 4.6). In order to avoid catalyst poisoning, sulphur must be removed to at least 1 ppmV before the gas passes to the fuel synthesis process [36, 38, 39]. Rectisol can efficiently remove acid compounds in the syngas as the achieved concentration of CO_2 and H_2S could be as low as 2 ppmV and 0.1 ppmV respectively [36]. IPSEpro does not include any models of absorption processes, thus a simple model was built which can be used as a general gas stream separation model. The model is shown in Figure 5-5. It is a single black-box model which includes separation efficencies for each component of the feed gas stream. The gas composition in the two exit streams of the model can be estimated by either setting the concentration for each component or prescribing the separation efficiencies. The same model was used to simulate the air separation unit. H_2S, HCl and CO_2 are removed together on top of the model, whereas the clean syngas exits from the bottom. H_2S and HCl concentrations in the clean syngas were set at 0.1ppmV (0.00001 vol%), whereas the CO_2 volume fraction was set at 2 % [90].

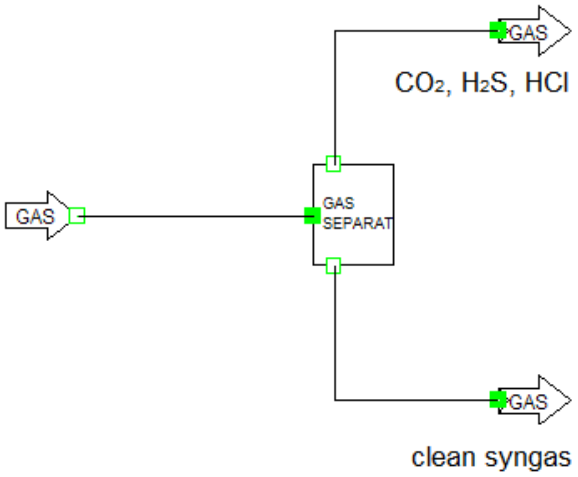

Figure 5-5: IPSEpro model of the Rectisol process

5.8 Gas cleaning & conditioning - EF gasifier

The gas cleaning section for the entrained flow gasifier is shown in Figure 5-10 in section 5.12.2.1. After gasification, the syngas is fed to a direct quench where it is cooled to the operating temperature of the WGS reactor (200^{o}C) [90]. The cooled syngas then passes through a bag filter to remove particulates. The H_2/CO ratio of the produced gas from the EF gasifier is 0.7, which is lower than the required ratio (H_2/CO = 2) for FT and methanol synthesis. Therefore, the ratio was adjusted by using a WGS reactor which was modelled at equilibrium conditions and had an exit gas temperature of 340°C [36]. The WGS reactor at this point of the process allows carbon dioxide produced from the WGS reactor to be removed soon after in the Rectisol unit. For the Rectisol process the same model with the CFB gasifier was used which was described in the previous section.

5.9 Fischer-Tropsch synthesis

5.9.1 Modelling approach

Just as with fast pyrolysis where a wide range of products is obtained, FT synthesis also yields a large number of different substances due to the low selectivity of the process (see also section 2.8.1.2). The number of individual chemical substances produced from FT

synthesis is very high, reaching a total of several hundred hydrocarbon species [5]. During FT synthesis many primary and secondary reactions take place leading to many individual components [147]. Detailed FT modelling is a task far beyond the time and resources in this study, thus some simplification was necessary. As with the fast pyrolysis model (see section 5.5), the FT synthesis model is based on a black-box approach. Neither chemical kinetics nor complex thermodynamic relationships were incorporated. The FT synthesis model was built to describe the mere relationship between syngas and FT hydrocarbon products in order to estimate the energy efficiency of the process and determine the products of interest.

In fast pyrolysis modelling a number of model substances were chosen to represent bio-oil in order to supply thermodynamic data necessary for the calculation of energy balances. The same approach was followed to model the liquid hydrocarbon products of FT synthesis.

Fürnsinn conducted a comprehensive and thorough research into the selection of representative model substances for the thermodynamic modelling of FT products on IPSEpro [5]. In his study only n-alkanes in the range of C_1 (methane) to C_{35} (penta-triacontane) were chosen. His selection of model substances for the FT products was mainly based on practical aspects regarding IPSEpro modelling (efficient integration of the model into IPSEpro) and on the following criteria [5]:

- Thermodynamic data such as heat capacity is not available for all FT products. Therefore, a selection of a specific number of representative model substances is unavoidable.
- Some products are more abundant than others; thus, products with low concentration such as highly branched hydrocarbons ($>C_{35}$), alkenes and alkanes isomers can be left out without significant effects on the results.
- Calculation times and programming efforts would highly increase if several hundred product substances were included.
- Reliable, quantitative data on the formation of the chosen model substances must be available; in practice, however, adequate data is scarce for many substance classes, let alone single product compounds.

- The chosen model substances should cover a wide range of FT products which include gases, gasoline, kerosene, diesel and waxes.

The chemical compounds selected by Fürnsinn are in good agreement with results reported in experimental studies of FT synthesis coupled with wood gasification. Sauciuc and Rauch found that for FT synthesis based on cobalt catalysts about 90% of the final FT products is alkanes [148]. This is also reported by CUTEC Institute [50] . Products such as alcohols, aldehydes, ketones, ethers, alkenes and alkanes isomers are 10% of the final FT products [148], thus these substances can be left out without significant effects on the mass and energy balances results. Additionally, C_1 to C_{35} alkanes cover the most abundant range of FT products [50, 54, 147] which include gases, gasoline, kerosene, diesel and waxes. Therefore, Fürnsinn's set of representative model substances for the thermodynamic modelling of FT products was selected for this study.

5.9.2 Thermodynamic modelling

The thermodynamic properties of methane (CH_4), ethane (C_2H_6) and propane (C_3H_8) have already been described by Pröll [126, 127] and are included in the PGP_Lib. Therefore, new mathematical relationships for the calculation of thermodynamic properties (ΔH_f, C_p) needed to be found for hydrocarbons from C_4 to C_{35}.

Enthalpy of formation

Similar to the thermodynamic modelling of fast pyrolysis (see section 5.5.2), since experimental values on thermodynamic properties (ΔH_f, C_p) of all selected model substances are not available, a mathematical function found in literature was used to estimate the enthalpy of formation for each model substance. To this end, the model of Helgeson [149] was used as, compared to other models [150-155], it is the most recent, has the most comprehensive applicability and fits well with experimental data. According to Helgeson's model, the standard enthalpy of formation can be calculated via a linear function of the carbon atoms of a n-alkane:

$$\Delta h^0_{f,298} = k_1 + k_2 \cdot n \qquad (5\text{-}21)$$

The values of the constants k_1 and k_2 depend on the substance class. For liquid n-alkanes these values are: k_1 = - 43.76 kJ/mol and k_2 = - 25.73 kJ/mol [149]. Note that the original

values are given in cal/mol but for this study they were converted to kJ/mol (1 cal = 4.184 J) as these units are used on IPSEpro for enthalpy calculations.

Heat capacity

For the heat capacity of liquid hydrocarbons, Helgeson's model could not be used as it is only valid for n>17. Therefore, the model of Durupt was used which fits well with experimental data [156]. Durupt proposes linear functions of temperature for the calculation of heat capacity of alkanes. Luria and Benson [157] propose more complex equations (cubic polynomials) but their results are similar to Durupt's model, thus Durupt's model was chosen instead. With Durupt's model, heat capacities of liquid alkanes are estimated using a group contribution approach, where values for the -CH_2- and -CH_3- groups are calculated to give the molecular heat capacity of an alkane [156]:

$$\text{CH}_2 \text{ group: } (C_p)_{CH_2} = 0.0354 \cdot T + 20.21$$

$$\text{CH}_3 \text{ group: } (C_p)_{CH_3} = 0.1205 \cdot T - 1.4721$$

Therefore, for a n-alkane (C_nH_{2n+2}) the heat capacity (J/mol·K) was calculated by the following equation:

$$C_p(T) = (n-2) \cdot (C_p)_{CH_2} + 2 \cdot (C_p)_{CH_3} \qquad (5\text{-}22)$$

Thus, the enthalpy of each model substance was calculated by the following equation:

$$\mathrm{H_i(T)} = \Delta \mathrm{h}^0_{\mathrm{f},298} + \int_{298.15}^{\mathrm{T}} C_p(T) \cdot dT \qquad (5\text{-}23)$$

$$= k_1 + k_2 \cdot n + \int_{298.15}^{\mathrm{T}} [(n-2) \cdot (0.0354 \cdot T + 20.21) + 2 \cdot (0.1205 \cdot T - 1.4721)]\, dT$$

$$= k_1 + k_2 \cdot n + \left[(n-2) \cdot \left(0.0354 \cdot \frac{T^2}{2} + 20.21 \cdot T \right) + 2 \cdot \left(0.1205 \cdot \frac{T^2}{2} - 1.4721 \cdot T \right) \right]_{298.15}^{T}$$

Similar to fast pyrolysis modelling, the total enthalpy of the FT hydrocarbon products was calculated as the weighted average of the enthalpies of the selected model substances (eqn. 5-9 at section 5.5.2.1). The mass fractions of the selected FT hydrocarbons were taken by the Anderson-Schultz-Flory product distribution (see section 2.8.1.2) for an alpha value of 0.85. This is further discussed in the following section. Due to the high number of

model substances the calculation of the total enthalpy was more complex than other processes modelled in this study. The calculation can be found in Appendix B.

5.9.3 Model structure

The model structure of the FT synthesis corresponds to a black-box approach. Figure 5-6 shows the model of FT synthesis which was built on IPSEpro for this study.

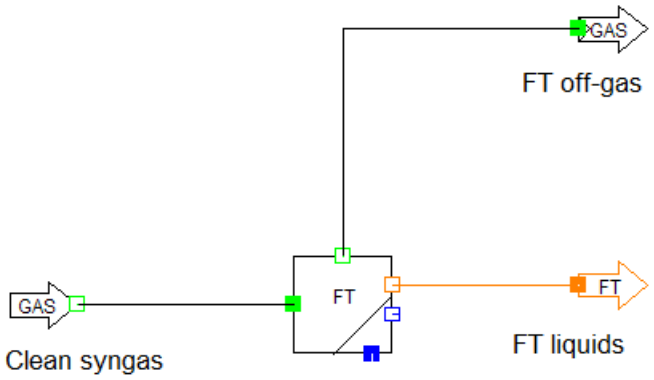

Figure 5-6: IPSEpro model of the Fischer-Tropsch synthesis

The black-box model includes reaction to FT hydrocarbons, product condensation and upgrading. Therefore, two product streams leave the model: FT off-gas on top and liquid hydrocarbons to the right. The FT off-gas consists of unconverted syngas and gaseous light hydrocarbons formed during the FT synthesis. It is assumed that the FT off-gas is sent to the power island for electricity production (once- through FT synthesis). Recycling of FT off-gas to the synthesis reactor via a reformer was not examined since it is claimed that the increased costs for reforming the light hydrocarbons of the FT off-gas exceed the benefits of increased fuel production [15, 88]. Furthermore, Tijmensen et al. [16] and Hamelick et al. [15] reported a small difference in energy efficiency between once-through operation and recycling of FT-off gas (2-3% higher for off-gas recycling). Once-through operation for FT synthesis also provides a significant second revenue stream from sale of electricity which can also be used to cover part of the electricity requirements of the plant.

The liquid FT hydrocarbons stream consists of all liquid FT products (gasoline, diesel, kerosene) and does not contain any dissolved light hydrocarbons or syngas. A description of the input and output streams of the FT synthesis model is given in Table 5-15.

The FT reaction is exothermic, thus a water cooling system (see section 5.5.4.1) was included in the model, which can be operated for steam generation. However, as discussed in section 4.8, a power plant was not modelled in this study so steam generation from fuel synthesis (FT and MTG) was not investigated.

As discussed in section 2.8.1.1, the low temperature Fischer-Tropsch synthesis (200 - 250^{o}C) favours the production of liquid fuels up to middle distillates. Therefore, the FT synthesis temperature was set to 230^{o}C. The operating pressure was set to 25 bar [48]. It should be noted that the Sasol Slurry Phase Distillate process, which is a low temperature Fischer-Tropsch synthesis, has similar operating conditions (see section 2.8.1.3).

Table 5-15: Input and output streams of the Fischer-Tropsch synthesis model

Input streams	**Characterisation**
Clean syngas	Gas composition (described in section 5.2.2)

Output streams	**Characterisation**
FT liquids	Elemental composition, enthalpy as a function of temperature based on model substances (section 5.9.2). They are divided into 4 product classes [158, 159]: • Gasoline All alkanes from C_5 to C_{12} • Kerosene All alkanes from C_{13} to C_{15} • Diesel Diesel products range from C_{16} to C_{19} • Wax All alkanes from C_{20} to C_{35}
FT off-gas	Gas composition (described in section 5.2.2)

5.9.4 Mass balances

As discussed in section 2.8.1.2, the Anderson-Schultz-Flory distribution is the most widely used model for the description of FT product distribution. As opposed to kinetic models

with much detail and complex calculation algorithms (e.g. Schulz/Claeys [160], Ahón et al. [161]), the ASF model is quite straightforward, as it only uses one parameter (the chain growth probability "α") for the calculation of the molar or mass fractions of the FT hydrocarbons. Furthermore, in accordance with the assumptions made in section 5.9.1, only linear alkanes are considered in the ASF model.

In this study, a chain growth probability value for the Anderson-Schultz-Flory distribution of 0.85 was chosen for estimation of the product composition based on reported literature values [5, 90, 147]. Figure 5-7 shows the ASF product distribution for an alpha value of 0.85.

At this chain growth probability, relatively low amounts of waxes are formed (approximately 19% - Figure 5-7), thus less wax products need to be hydrocracked [5]. Following Swanson [90], Furnsinn [5] and Hamelinck [15], it was assumed that after FT synthesis all waxes are hydrocracked to middle distillate products (C_{10}-C_{19}). The product from the hydrocracking unit is isomerised to improve the cold flow properties and subsequently fractionated in a conventional distillation column, as discussed in section 2.8.1.2. A product distribution of 60% diesel, 25% gasoline and 25% kerosene was assumed for the hydrocracking unit, as reported from Eilers et al. [49] for the SMDS process (see section 2.8.1.3).

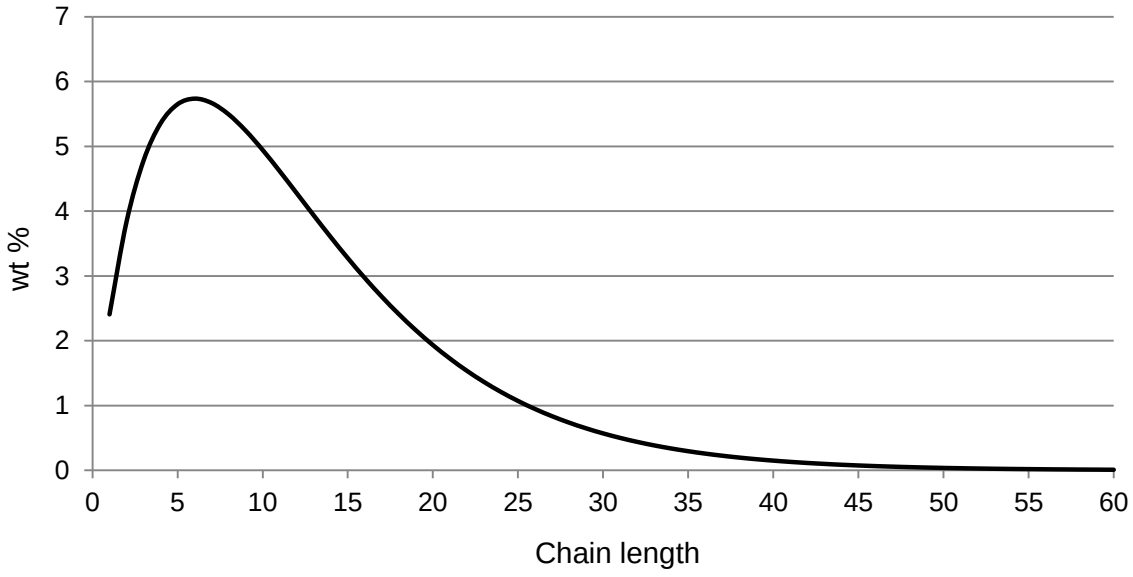

Figure 5-7: ASF product distribution for α=0.85

Hydrocracking of FT hydrocarbons was not modelled on IPSEpro due to time constraints and to avoid complexity. However, it was considered in the economic assessment and its capital and operating costs were included in the cost estimations.

The FT synthesis model employs elemental mass balances of all components entering and leaving the model in order to estimate the relative amount of products formed. Similar to other IPSEpro models of the PGP_Lib (e.g. biomass gasifier), the elemental mass balances were set up for carbon (C), hydrogen (H), oxygen (O), nitrogen (N), argon (Ar), sulphur (S) and chlorine(Cl).

The elemental composition of the FT liquids stream (see Table 5-15) was estimated in the model from the following equations:

$$wC + wH = 1 \qquad (5\text{-}24)$$

$$\frac{wC}{wH} = \frac{12.011 \cdot n}{1.00794 \cdot (2 \cdot n + 2)} \qquad (5\text{-}25)$$

where wC and wH are the weight fractions (kg/kg) of carbon and hydrogen of the FT liquid mix, 12.011 and 1.00794 is the atomic weight (g/mol) of carbon and hydrogen, respectively. The chain length n for the selected FT alkanes (general formula: C_nH_{2n+2}) is a variable of the model and needs to be set by the user. It was calculated as the weighted average of the chain lengths of the selected model substances:

$$\bar{n} = \sum n_i \cdot x_i \qquad (5\text{-}26)$$

where x_i is the mass fraction of each model substance from the ASF product distribution as shown in Figure 5-7. Note that the mass fractions of the remaining C_{35+} hydrocarbons (about 2 wt% in total) are added to C_{35} for calculating the average n.

5.9.5 Energy balance

The energy balance equation was similar to that of the other IPSEpro models already described in this study:

$$\dot{h}(syngas) = \dot{h}(FT\ off\text{-}gas) + \dot{h}(FT\ liquids) + Q_{clg} \cdot 3600 + Q_{loss} \cdot 3600 \qquad (5\text{-}27)$$

5.9.6 Fischer-Tropsch model variables

Several variables were required to describe the FT synthesis model. These are briefly described in Table 5-16.

Table 5-16: Variables of the FT synthesis model

Variable	Unit	Description
dp_gas	bar	Pressure difference between syngas and FT off-gas
dp_FTliq	bar	Pressure difference between syngas and FT liquids
dp_clg	bar	Pressure drop of the cooling stream
dt_gas	^{o}C	Temperature difference between syngas and FT off-gas
dt_FTliq	^{o}C	Temperature difference between syngas and FT liquids
n	-	Average chain length of FT liquid products (eqn.5-26)
Q_clg	kW	Cooling duty of the reactor heat exchanger
Q_loss	kW	Heat loss from the reactor

5.10 Methanol synthesis and Methanol-to-Gasoline (MTG)

5.10.1 Modelling approach

As with FT synthesis, a simplified approach was also used to model the MTG process. In contrast to the abundant literature for FT synthesis, there is a dearth of published literature for the methanol-to-gasoline (MTG) process. This made the modelling task more difficult compared to other processes modelled in this study and also increased the uncertainty in the results. The MTG process also produces a wide range of chemical substances (see section 2.8.2.2). Quantitative data on the formation of products is scarce for many substance classes and especially for single product compounds. Therefore, simplification was once again necessary.

The main product of the MTG process is gasoline at approximately 80 wt % [59, 65]. As already discussed in the previous sections (5.5.1 and 5.9.1), a set of model substances had to be defined in order to estimate the thermodynamic properties of the gasoline product. Table 5-17 shows the different substance classes composition in gasoline.

Table 5-17: MTG gasoline composition [162]

Substance class	wt %
Alkanes	60
Alkenes	12
Aromatics	28

The reasons for the selection of the model substances were similar to the FT synthesis and fast pyrolysis and were discussed in the previous sections (5.5.1 and 5.9.1). Quantitative data on the formation of single compounds could not be found in the literature thus, as with fast pyrolysis, a model substance representative of the substance classes shown in Table 5-17 was selected. The selection was based on the availability of thermodynamic data of the gasoline products. Table 5-18 shows the three representative model compounds of gasoline selected in this study.

Table 5-18: MTG gasoline model substances

Substance class	Compound	wt %
Alkanes	Heptane	60
Alkenes	Octene	12
Aromatics	Benzene	28

5.10.2 Thermodynamic modelling

The thermodynamic properties of methanol and DME were estimated using the Joback method which was described in section 5.5.2. With regards to the MTG gasoline, for the estimation of enthalpy of each model substance in both the gaseous and liquid gasoline, the NASA-polynomials by Burcat and McBride [163] were used. NASA-polynomials were also used by Pröll [126] to calculate the enthalpy of gas compounds of the PGP_Lib.

For enthalpy calculations, the isobaric heat capacity is needed whose temperature dependency $C_p(T)$ is described by the 5-coefficient dimensionless NASA-polynomials [164]:

$$\frac{C_p(T)}{R} = a_1 + a_2 \cdot T + a_3 \cdot T^2 + a_4 \cdot T^3 + a_5 \cdot T^4 \qquad (5\text{-}28)$$

From equation 5-1 and equation 5-28, the NASA-polynomial for enthalpy is given by the following equation [127]:

$$\frac{H_i(T)}{R} = a_1 \cdot T + \frac{a_2}{2} \cdot T^2 + \frac{a_3}{3} \cdot T^3 + \frac{a_4}{4} \cdot T^4 + \frac{a_5}{5} \cdot T^5 + a_6 \qquad (5\text{-}29)$$

where *R* is the gas constant (8.314 J/mol·K). Burcat and McBride [163] report the coefficients a_1-a_6 for a large number of substances, where they distinguish two parameter sets for low (≤1000 K) and high (>1000 K) temperatures. Table 5-19 shows the coefficients a_1-a_6 of the NASA polynomials for the selected model substances.

Table 5-19: NASA-polynomials coefficients for the selected model substances in gaseous (G) and liquid (L) gasoline [163]

Compound	a_1	a_2	a_3	a_4	a_5	a_6
Heptane (G)	1.75E+1	4.21E-2	-1.64E-5	2.99E-9	-2.06E-13	-3.17E+4
Heptane (L)	3.58E+1	-1.4E-1	4.92E-4	-4.04E-7	0	-3.5E+4
Octene (G)	2.08E+1	3.83E-2	-1.24E-5	-1.8E-9	-9.37E-14	-2.02E+4
Octene (L)	2.60E+1	6.43E-2	9.25E-06	-5.1E-8	2.33E-11	-1.36E+4
Benzene (G)	1.18E+1	1.91E-2	-6.54E-6	9.8E-10	-5.33E-14	4.07E+3
Benzene (L)	6.37E+1	-6E-1	2.67E-3	-5.06E-6	3.64E-9	-1.67E+3

Similar to fast pyrolysis and FT modelling, the total enthalpy of the MTG gasoline was calculated as the weighted average of the enthalpies of the selected model substances (eqn. 5-9 at section 5.5.2.1).

5.10.3 Model structure

As with FT synthesis and fast pyrolysis, the IPSEpro model of the methanol synthesis and MTG process was kept as simple as possible in order to ensure a working and effective model. Thus no chemical kinetics or complex thermodynamic relationships were included. The IPSEpro model of methanol synthesis and the MTG process is shown in Figure 5-8. Syngas from gas clean-up passes to the methanol synthesis reactor where it is converted to methanol at 50 bar and 250^{o}C [60, 61]. The crude methanol is then fed to the MTG plant.

The simulation of the MTG process (process layout, operating conditions) was based on the ExxonMobil's MTG plant [59, 65]. Methanol is vaporised by heat exchange with MTG reactor effluent gases before it enters the DME reactor where a mixture of DME, methanol and water is produced at 404^{o}C.

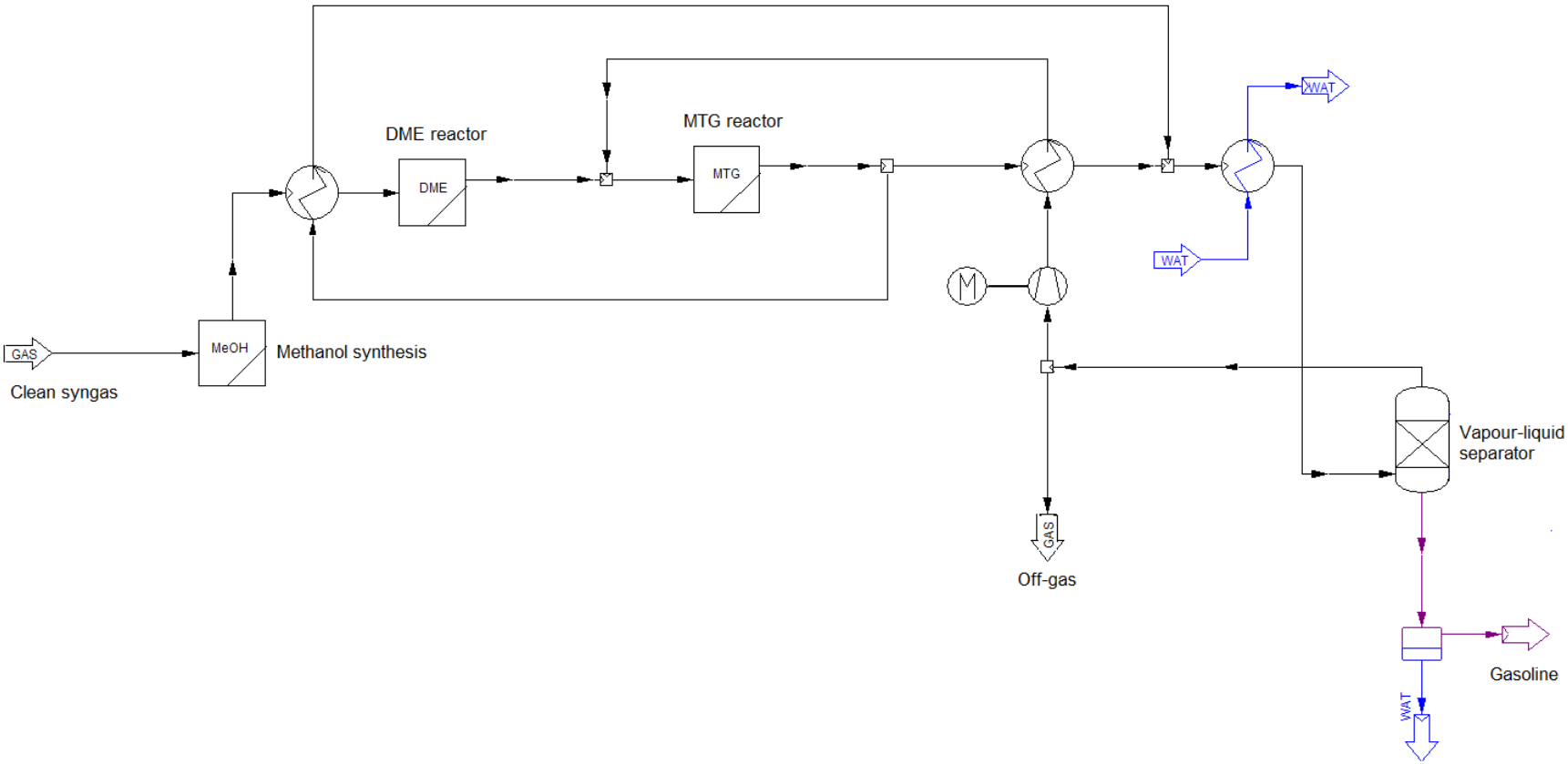

Figure 5-8: IPSEpro model of the methanol synthesis and MTG process

The effluent from the DME reactor is combined with recycle gas from the product separator and enters the MTG reactor where it is converted at 415^{o}C and 21.2 bar to mainly hydrocarbons and water.

The hot reactor effluent is cooled by heat exchange with recycle gas from the vapour-liquid separator. It is then further cooled to about 200^{o}C before it passes to the vapour-liquid separator, where gas, liquid gasoline and water separate. The off-gas from the product separator contains mostly low hydrocarbons (C_1-C_3), CO and CO_2. The water from the product separator contains trace amounts of oxygenated organic compounds and thus it requires treatment [58].

5.10.4 Mass and energy balances

Methanol synthesis

Methanol synthesis catalysts have been reported to be extremely selective, with 99% or better selectivity to methanol [60]. According to LeBlanc et al. [60], methanol synthesis by-products are present in concentrations of less than 5000 ppmw and they are also reported to be converted by the downstream MTG process [92]. Therefore, given the high selectivity reported in the literature, no other by-products (e.g. higher alcohols, hydrocarbons) were included in the crude methanol product.

The elemental composition of methanol was set in IPSEpro to 37.5% carbon, 12.5% hydrogen and 50% oxygen and was calculated from the molecular weights of the individual elements (C, H, O) in methanol (CH_4O, M=32 g/mol). An example is given for hydrogen:

$$wt\%\ H = \frac{4 \cdot 1.00794}{32} \cdot 100 = 12.5$$

Philips [92] reports 96 wt% methanol purity in the product, whereas Jones [94] assumes 93 wt%. In the ExxonMobil's MTG plant (see section 2.8.2.2), methanol at 83 wt% was produced [60]. In this study, it was assumed that methanol at 90% purity was produced which is the approximate average of the reported literature values. The other 10% mainly consists of H_2O, CO and CO_2.

DME reactor

In order to estimate the elemental composition and product yield of the DME reactor effluent, the conversion of methanol to DME and H_2O was set in the model to 77% [65]. The elemental composition of the oxygenate product mix (DME and methanol) estimated in the model was 47.5% carbon, 12.8% hydrogen and 39.7% oxygen.

MTG reactor

For the MTG reactor, the gasoline fraction in the product stream was set to 36 wt% of the methanol and DME input as reported by Yurchac [65] for the ExxonMobil MTG process. The conversion of methanol and DME was 100% [58, 65, 162] thus the product stream did not contain any methanol or DME. The gasoline's composition estimation was based on the three selected model substances and their respective weight fractions (see Table 5-18 at section 5.10.1). For example the weight fraction for carbon of the gasoline product was given by the following equation:

$$w_{c,gasoline} = w_{alkanes} \cdot w_{c,alkanes} + w_{alkenes} \cdot w_{c,alkenes} + w_{aromatics} \cdot w_{c,aromatics} \quad (5\text{-}30)$$
$$= w_{heptane} \cdot w_{c,heptane} + w_{octene} \cdot w_{c,octene} + w_{benzene} \cdot w_{c,benzene}$$

where w_i is the weight fraction of the model substance, and $w_{c,i}$ is the weight fraction of carbon in the model substance. A similar equation was used for hydrogen. The elemental composition of gasoline estimated in the model was 86% carbon and 14% hydrogen.

Energy balances were similar to the other IPSEpro models described in this study. Energy balances for each individual model of the overall methanol synthesis and MTG model are given by the following equations:

Methanol synthesis:

$$\dot{h}(syngas) = \dot{h}(methanol + other\ gases) + Q_{clg} \cdot 3600 + Q_{loss} \cdot 3600 \quad (5\text{-}31)$$

DME reactor:

$$\dot{h}(methanol + other\ gases) =$$
$$\dot{h}(DME + methanol + other\ gases) + Q_{clg} \cdot 3600 + Q_{loss} \cdot 3600 \quad (5\text{-}32)$$

MTG reactor:

$$\dot{h}(DME + methanol + other\ gases) =$$

$$\dot{h}(gasoline + other\ gases) + Q_{clg} \cdot 3600 + Q_{loss} \cdot 3600 \quad (5\text{-}33)$$

5.11 Topsoe Integrated Gasoline Synthesis (TIGAS)

5.11.1 Modelling approach and model structure

There is even less information in the literature about the TIGAS process than the MTG process. As discussed in section 4.7, numerous efforts were made to get cost and performance data from industrial contacts at Haldor Topsoe but without success. Information about the product distribution and the operating conditions of the gasoline synthesis reactor of the TIGAS process could not be found. Therefore, for modelling purposes, it was assumed that the TIGAS gasoline had the same composition with the MTG gasoline which was described in the previous section.

The IPSEpro model of the TIGAS process is shown in Figure 5-9. As already discussed in sections 2.8.3 and 4.7, the main difference between the TIGAS process and the MTG process is the absence of a discrete methanol synthesis step. In the TIGAS process, methanol and DME are synthesised in one reactor (oxygenate synthesis reactor) and they are then converted to gasoline in the gasoline synthesis reactor (same as the MTG reactor [58]). For the TIGAS oxygenate reactor, the DME reactor model which was built for the MTG process was used with some minor changes that are discussed in the next section. Both the TIGAS oxygenate reactor and MTG's DME reactor produce methanol and DME thus there was no need to build a different model. As with the MTG process, the gasoline product is separated from gas and water in a vapour-liquid separator.

5.11.2 Mass and energy balances

In order to estimate the elemental composition and product yield of the oxygenate synthesis reactor effluent, the weight fraction of methanol and DME in the oxygenate product mix were set in the model to 20% and 80%, respectively [70].

The gasoline synthesis reactor of the TIGAS process used the same technology with the gasoline synthesis reactor of the MTG process [58]. Therefore, the model settings of the TIGAS gasoline reactor were the same with the MTG reactor (see section 5.10.4).

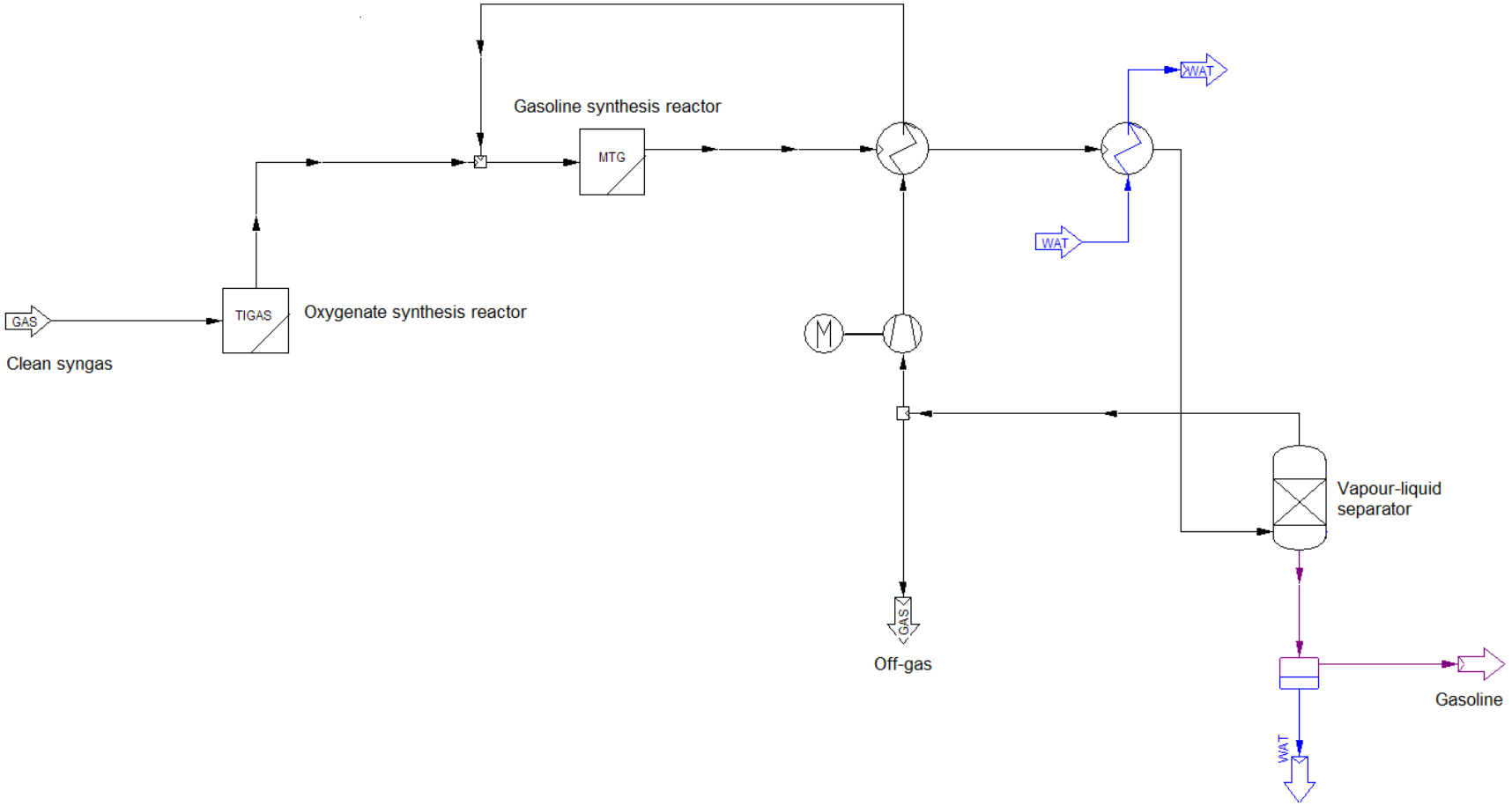

Figure 5-9: IPSEpro model of the TIGAS process

Energy balances were similar to the MTG process models. Energy balances for each individual model of the TIGAS model are given by the following equations:

Oxygenate synthesis reactor:

$$\dot{h}(syngas) = \dot{h}(DME + methanol + other\ gases) + Q_{clg} \cdot 3600 + Q_{loss} \cdot 3600 \qquad (5\text{-}34)$$

Gasoline synthesis reactor:

$$\dot{h}(DME + methanol + other\ gases) =$$
$$\dot{h}(gasoline + other\ gases) + Q_{clg} \cdot 3600 + Q_{loss} \cdot 3600 \qquad (5\text{-}35)$$

5.12 Results

In the following sections the results of the performance assessment are presented, starting with the definition of the energy conversion efficiency of a BTL plant used in this study. The performance results and the flow sheets of the different BTL concepts are presented and a comparison is later made between the modelled BTL concepts.

5.12.1 Definition of energy efficiency

The energy conversion efficiency is widely used to measure the technical performance and the economic feasibility of chemical plants. The energy efficiency of a BTL plant is a measure as to which extent the biomass energy remains in the hydrocarbon fuels products. In this study, it is defined as the ratio between the total energy in the hydrocarbon fuels output and that in the biomass feedstock:

$$\eta_{plant} = \frac{\dot{M}_{fuels} \cdot LHV_{fuels}}{\dot{M}_{biomass} \cdot LHV_{dry\ biomass}} \qquad (5\text{-}36)$$

where $\dot{M}_{fuels}$ is the mass flow (kg/h) of hydrocarbon fuels, LHV_{fuels} is the lower heating value (kJ/kg) of hydrocarbon fuels, $\dot{M}_{biomass}$ is the mass flow input (kg/h) of the daf biomass and $LHV_{biomass}$ is the lower heating value (kJ/kg) of the daf biomass feed. The energy efficiency as defined above was calculated for each selected BTL plant concept in order to compare the different BTL concepts in terms of performance.

5.12.2 BTL concepts based on biomass gasification

Each process step was described in detail in the previous sections so a summary of the nine BTL concepts will be provided here. The selected BTL concepts are summarised in Table 4-1 in section 4.9.

5.12.2.1 EF-FT concept

The flowsheet of the EF-FT concept is shown in Figure 5-10. The EF-FT concept included entrained flow gasification and Fischer-Tropsch synthesis as already discussed in section 4.9. After drying to 10% water content, biomass was gasified in an entrained flow reactor at 1400^{o}C. The produced gas was then quenched and scrubbed of particulates as discussed in section 5.8. A WGS reactor was employed to adjust the H_2/CO ratio of the syngas to the required consumption ratio for FT synthesis. Hydrogen sulphide and carbon dioxide when then removed in the Rectisol unit and the clean syngas passed to the FT synthesis to produce liquid hydrocarbon fuels.

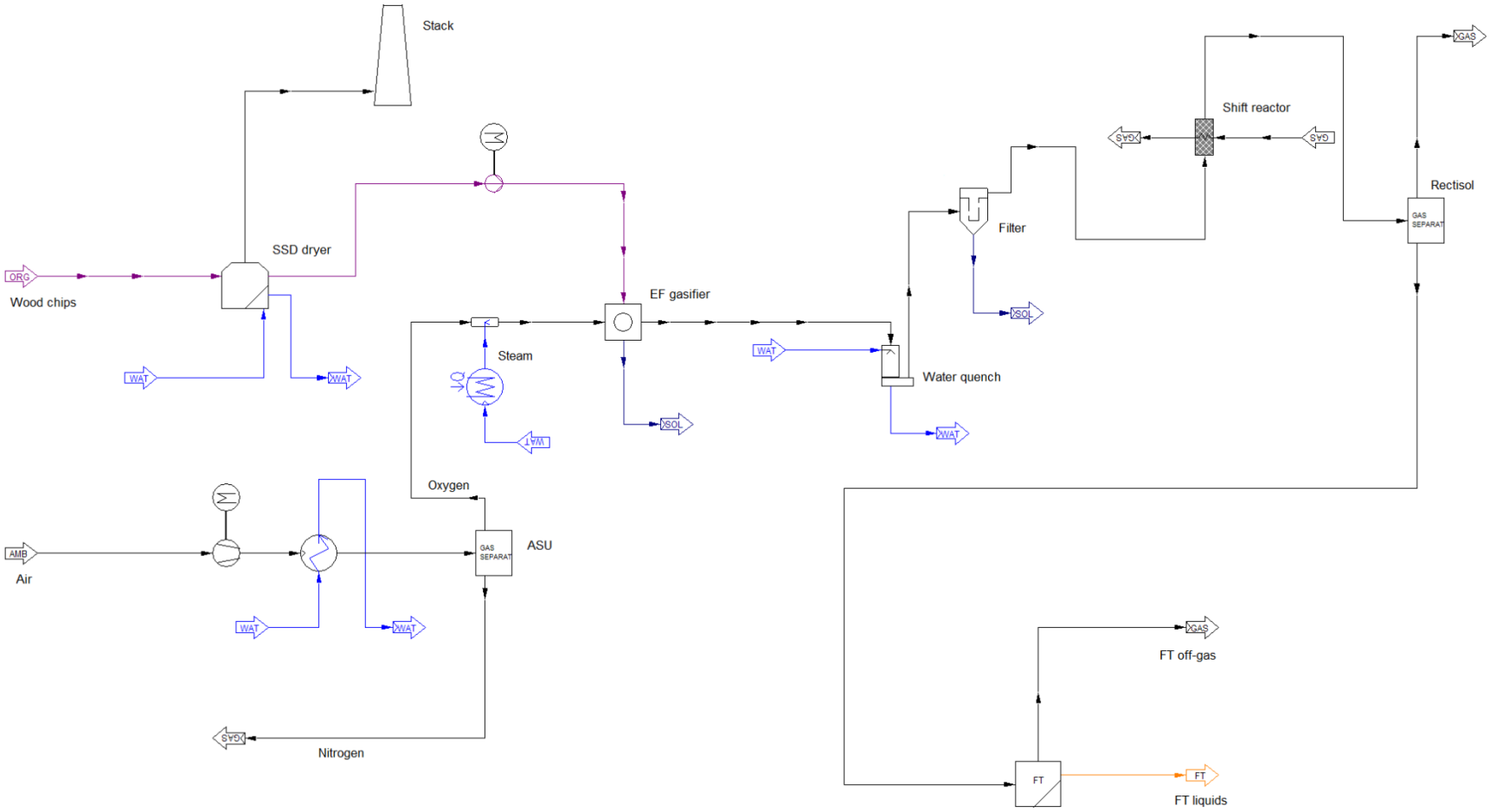

Figure 5-10: Flow sheet of the EF-FT process concept

Table 5-20 shows the results of the IPSEpro simulation analysis of the EF- FT concept. Looking at the energy conversion efficiency of this concept, which correlates the energy of the FT hydrocarbon fuels and the energy in biomass, 45% of this energy is recovered in the FT fuels. This is mainly due to the high amount of produced off-gas in the FT synthesis which also contains unconverted syngas.

Table 5-20: Settings and results of the EF-FT concept simulation

Biomass		
LHV wet biomass	kJ/kg	13,056
Water content	%	30
Mass flow (wet)	kg/h	120,000
LHV daf biomass	kJ/kg	19,897
Mass flow (dry)	kg/h	84,000
Mass flow (dry)	t/d	2016
FT-fuels		
LHV	kJ/kg	43,917
HHV	kJ/kg	47,276
Mass flow	kg/h	16,958
Mass flow	t/d	406.9
FT-off gas		
Mass flow	kg/h	42,237
Energy efficiency (eqn. 5-36)	%	45
FT-fuels mass yield (daf basis)	%	20.4

5.12.2.2 CFB-FT concept

The CFB-FT concept differs from the EF-FT concept by the gasification and gas cleaning steps. The flow sheet of the CFB-FT concept is shown in Figure 5-11. Instead of an entrained flow gasifier, a CFB gasifier was employed with subsequent gas cleaning technologies including tar cracking, particulates and acid gas removal as discussed in section 5.7. The results of the simulation analysis of the CFB-FT concept are shown in Table 5-21.

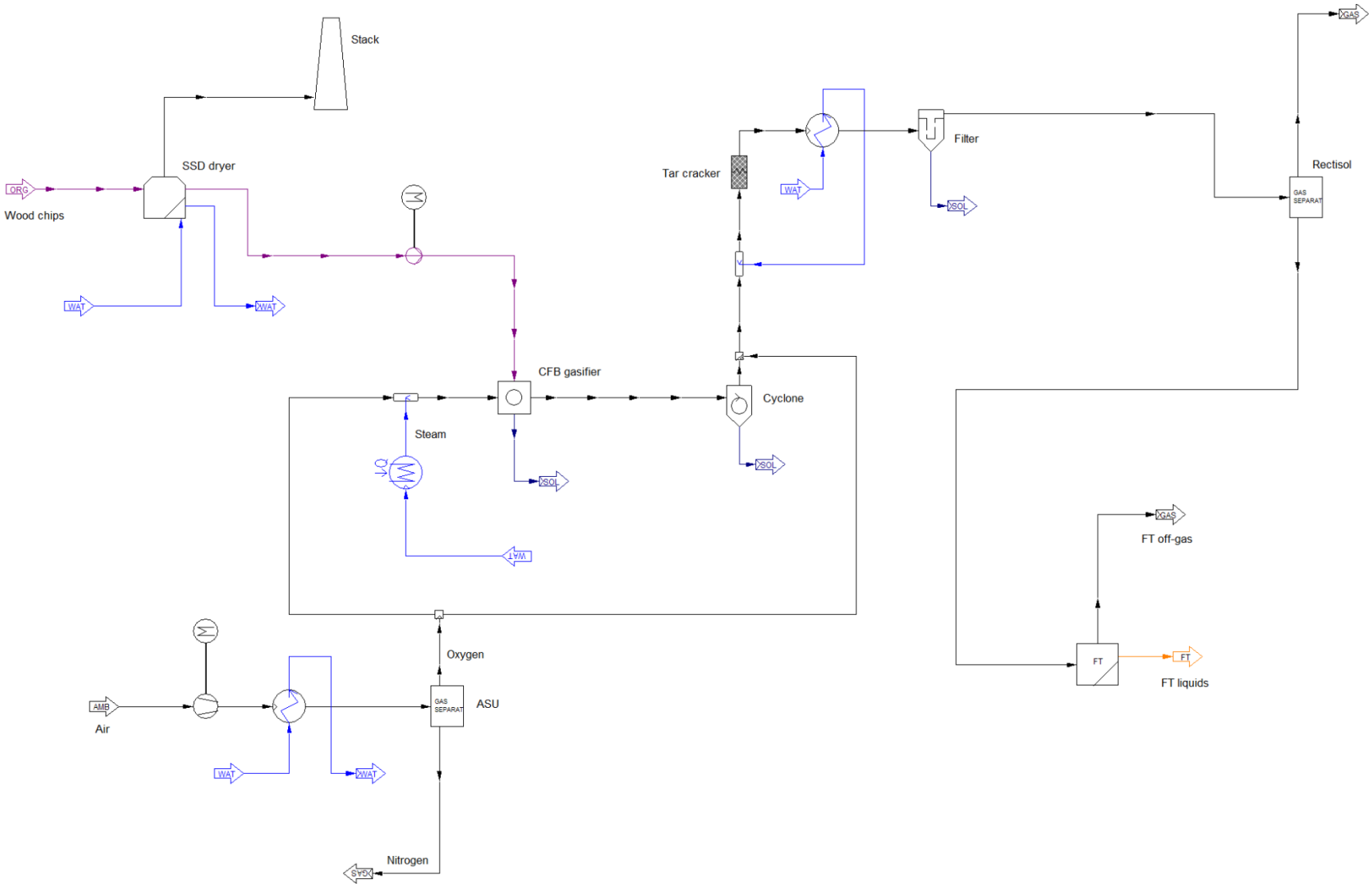

Figure 5-11: Flow sheet of the CFB-FT process concept

Table 5-21: Settings and results of the CFB-FT concept simulation

Biomass		
LHV wet biomass	kJ/kg	13,056
Water content	%	30
Mass flow (wet)	kg/h	120,000
LHV daf biomass	kJ/kg	19,897
Mass flow (dry)	kg/h	84,000
Mass flow (dry)	t/d	2016
FT-fuels		
LHV	kJ/kg	43,917
HHV	kJ/kg	47,276
Mass flow	kg/h	17,930
Mass flow	t/d	430.3
FT-off gas		
Mass flow	kg/h	48,860
Energy efficiency (eqn. 5-36)	%	47.6
FT-fuels mass yield (daf basis)	%	21.6

5.12.2.3 EF-MTG concept

The MTG process was used as the fuel synthesis technology for the EF-MTG concept instead of FT synthesis which was employed in the previous two concepts. The gasification and gas cleaning steps were the same with the EF-FT concept. Figure 5-12 shows the IPSEpro flow sheet of the EF-MTG concept. The results of the simulation analysis of this concept are shown in Table 5-22. It should be noted that the energy efficiency of the EF-MTG concept is lower than the energy efficiencies of the previous FT based concepts. This is further discussed in section 5.12.4, where a comparison between the modelled concepts is made.

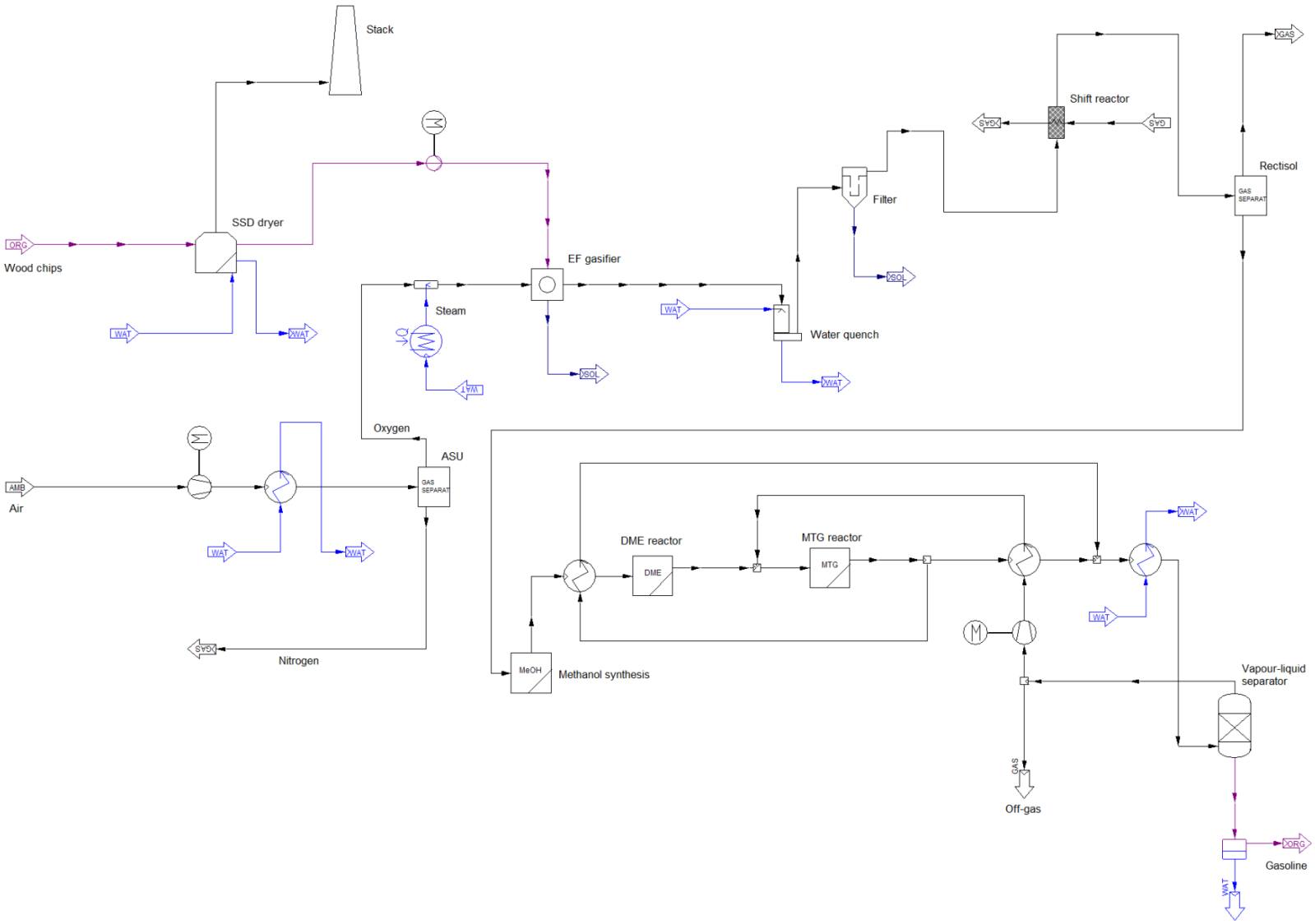

Figure 5-12: Flow sheet of the EF-MTG process concept

Table 5-22: Settings and results of the EF-MTG concept simulation

Biomass		
LHV wet biomass	kJ/kg	13,056
Water content	%	30
Mass flow (wet)	kg/h	120,000
LHV daf biomass	kJ/kg	19,897
Mass flow (dry)	kg/h	84,000
Mass flow (dry)	t/d	2016
MTG gasoline		
LHV	kJ/kg	42,308
HHV	kJ/kg	45,354
Mass flow	kg/h	14,810
Mass flow	t/d	355.4
MTG-off gas		
Mass flow	kg/h	19,149
Energy efficiency (eqn. 5-36)	%	37.9
Gasoline mass yield (daf basis)	%	17.8

5.12.2.4 CFB-MTG concept

For this concept, CFB gasification and the MTG process were employed. The CFB gasification and the subsequent gas cleaning steps were kept the same with the CFB-FT concept. The flow sheet of the CFB-MTG process is shown in Figure 5-13, whereas the simulation results are shown in Table 5-23.

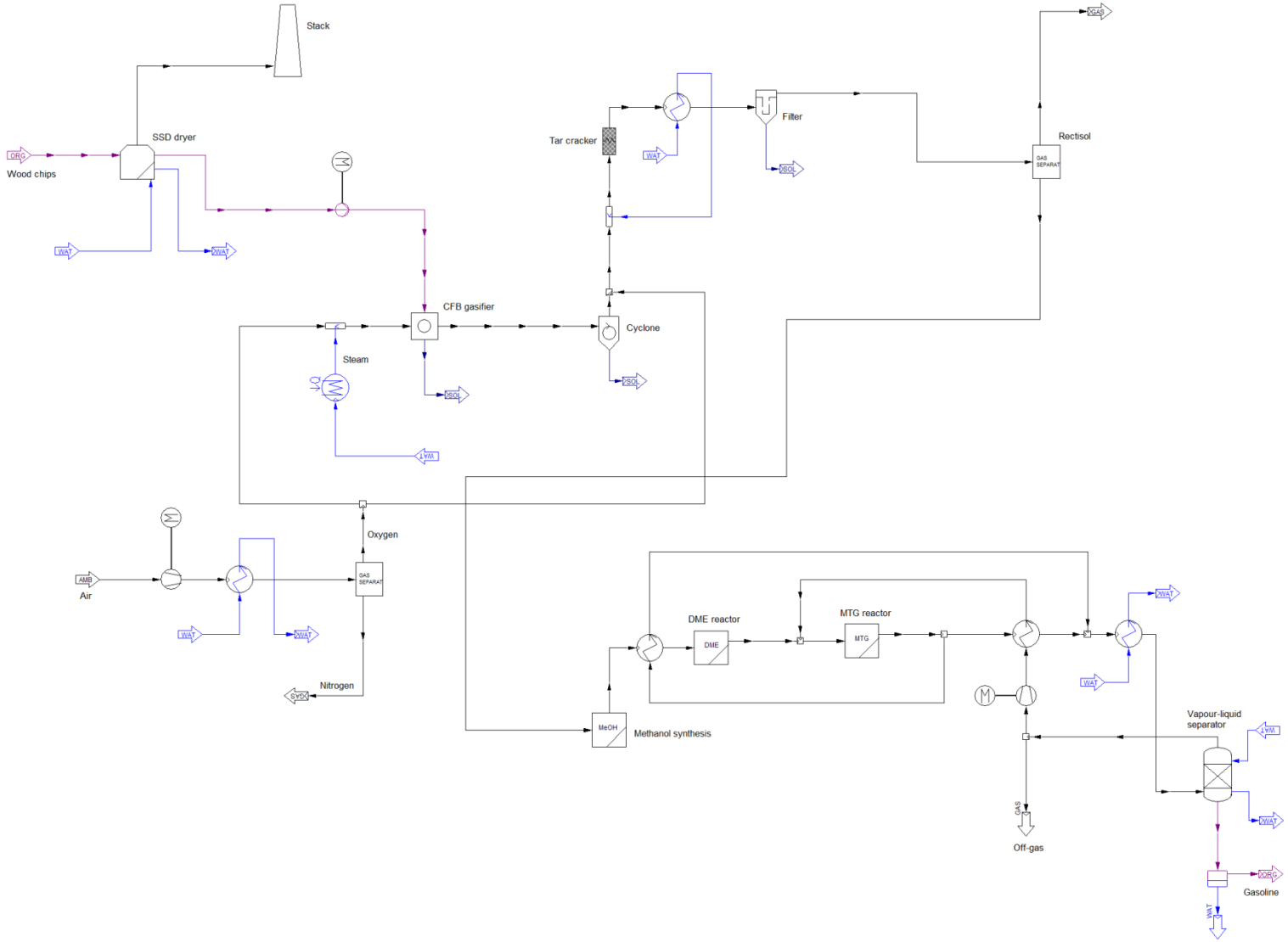

Figure 5-13: Flow sheet of the CFB-MTG process concept

Table 5-23: Settings and results of the CFB-MTG concept simulation

Biomass		
LHV wet biomass	kJ/kg	13,056
Water content	%	30
Mass flow (wet)	kg/h	120,000
LHV daf biomass	kJ/kg	19,897
Mass flow (dry)	kg/h	84,000
Mass flow (dry)	t/d	2016
MTG gasoline		
LHV	kJ/kg	42,307
HHV	kJ/kg	45,353
Mass flow	kg/h	16,980
Mass flow	t/d	407.5
MTG-off gas		
Mass flow	kg/h	19,137
Energy efficiency (eqn. 5-36)	%	43.4
Gasoline mass yield (daf basis)	%	20.4

5.12.2.5 EF-TIG concept

The EF-TIG employed a different fuel synthesis technology to the other concepts, the TIGAS process. The gasification and gas cleaning steps were the same with the other EF based concepts to retain consistency and to make results comparable. The flow sheet of the EF-TIG concept is shown in Figure 5-14. Table 5-24 shows the results of the simulation analysis of the EF-TIG concept on IPSEpro.

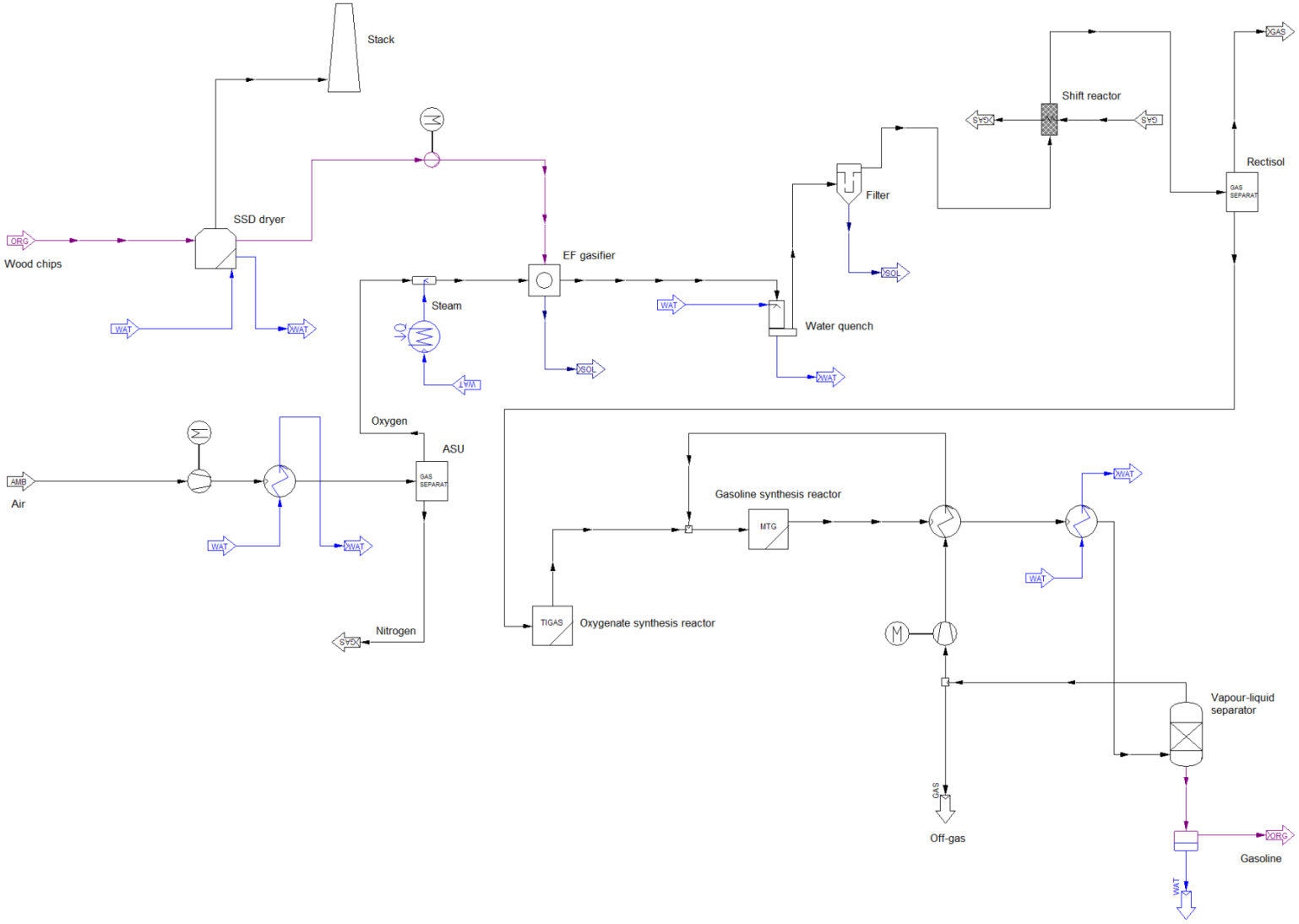

Figure 5-14: Flow sheet of the EF-TIG process concept

Table 5-24: Settings and results of the EF-TIG concept simulation

Biomass		
LHV wet biomass	kJ/kg	13,056
Water content	%	30
Mass flow (wet)	kg/h	120,000
LHV daf biomass	kJ/kg	19,897
Mass flow (dry)	kg/h	84,000
Mass flow (dry)	t/d	2016
TIGAS gasoline		
LHV	kJ/kg	42,338
HHV	kJ/kg	45,383
Mass flow	kg/h	15,831
Mass flow	t/d	379.9
TIGAS-off gas		
Mass flow	kg/h	17,398
Energy efficiency (eqn. 5-36)	%	40.5
Gasoline mass yield (daf basis)	%	19

5.12.2.6 CFB-TIG concept

This concept was similar to the previous CFB based concepts although the TIGAS process was employed for the production of synthetic hydrocarbon fuels. The IPSEpro flow sheet of the CFB-TIG concept is shown in Figure 5-15. Table 5-25 shows the results of the simulation analysis of this TIGAS based concept. It should be noted that both TIGAS based concepts give higher energy efficiencies than the MTG based concepts but lower efficiencies than the FT based concepts. This is further discussed in section 5.12.4.

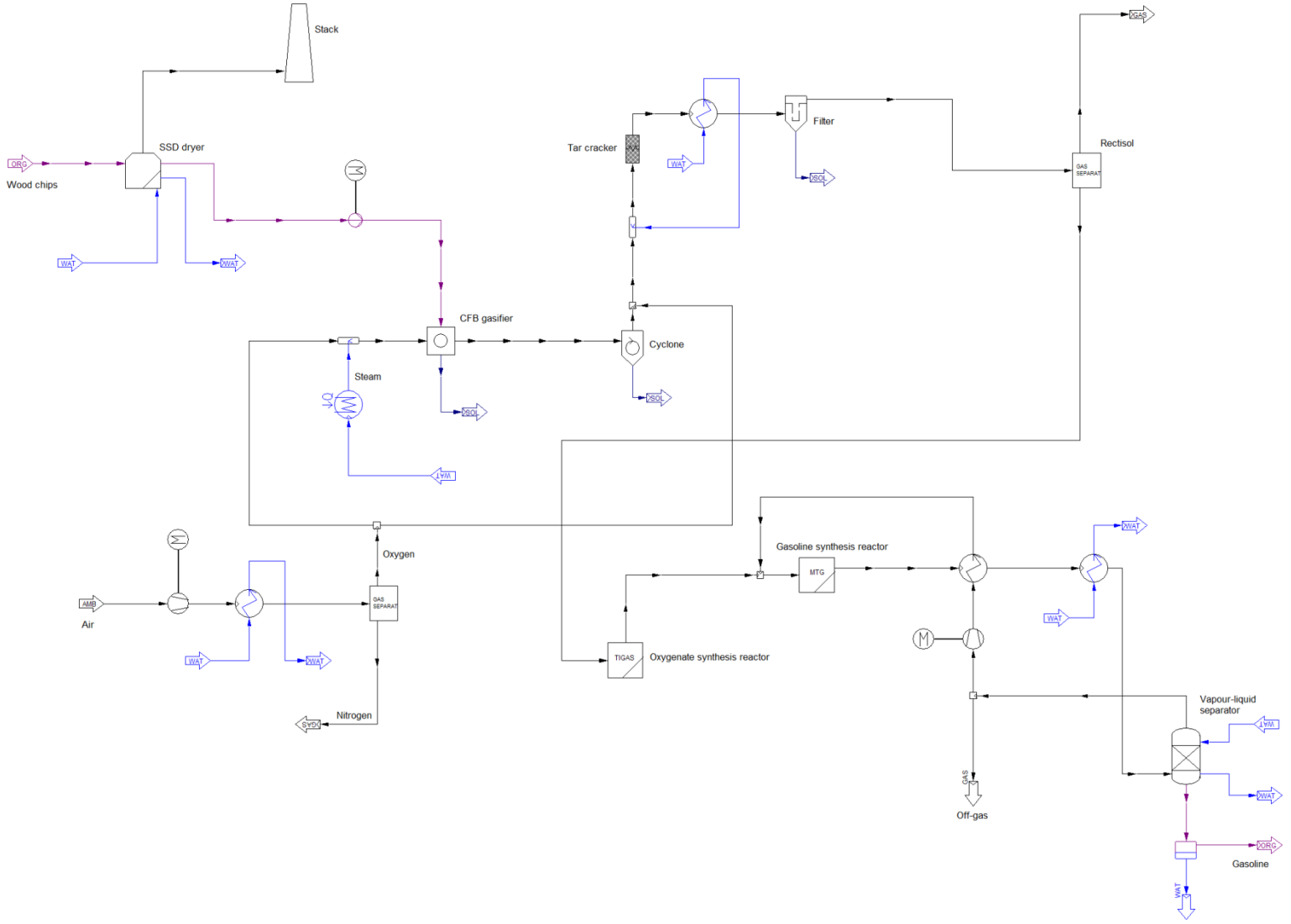

Figure 5-15: Flow sheet of the CFB-TIG process concept

Table 5-25: Settings and results of the CFB-TIG concept simulation

Biomass		
LHV wet biomass	kJ/kg	13,056
Water content	%	30
Mass flow (wet)	kg/h	120,000
LHV daf biomass	kJ/kg	19,897
Mass flow (dry)	kg/h	84,000
Mass flow (dry)	t/d	2016
TIGAS gasoline		
LHV	kJ/kg	42,312
HHV	kJ/kg	45,358
Mass flow	kg/h	17,541
Mass flow	t/d	420.9
TIGAS-off gas		
Mass flow	kg/h	17,828
Energy efficiency (eqn. 5-36)	%	44.9
Gasoline mass yield (daf basis)	%	21

5.12.3 BTL concepts based on bio-oil gasification

In this section the results of the simulation analysis of the BTL concepts based on bio-oil gasification are presented. As discussed in section 4.4, fast pyrolysis was employed as an alternative to energy intensive and costly biomass grinding for the entrained flow gasification based concepts. The evaluation of fast pyrolysis as a pretreatment option for entrained flow gasification also allowed for the comparison of BTL concepts based on bio-oil gasification with BTL concepts based on solid biomass gasification. The fast pyrolysis model used in the bio-oil gasification concepts was described in section 5.5.

5.12.3.1 FP-FT

As discussed in section 4.4, five regional pyrolysis plants with a capacity of 400 dry t/d each, supplied a central BTL plant with bio-oil. In the IPSEpro model shown in Figure 5-16, the five fast pyrolysis plants were represented as one fast pyrolysis plant for a more efficient integration into IPSEpro (lower calculation times, lower overall model complexity).

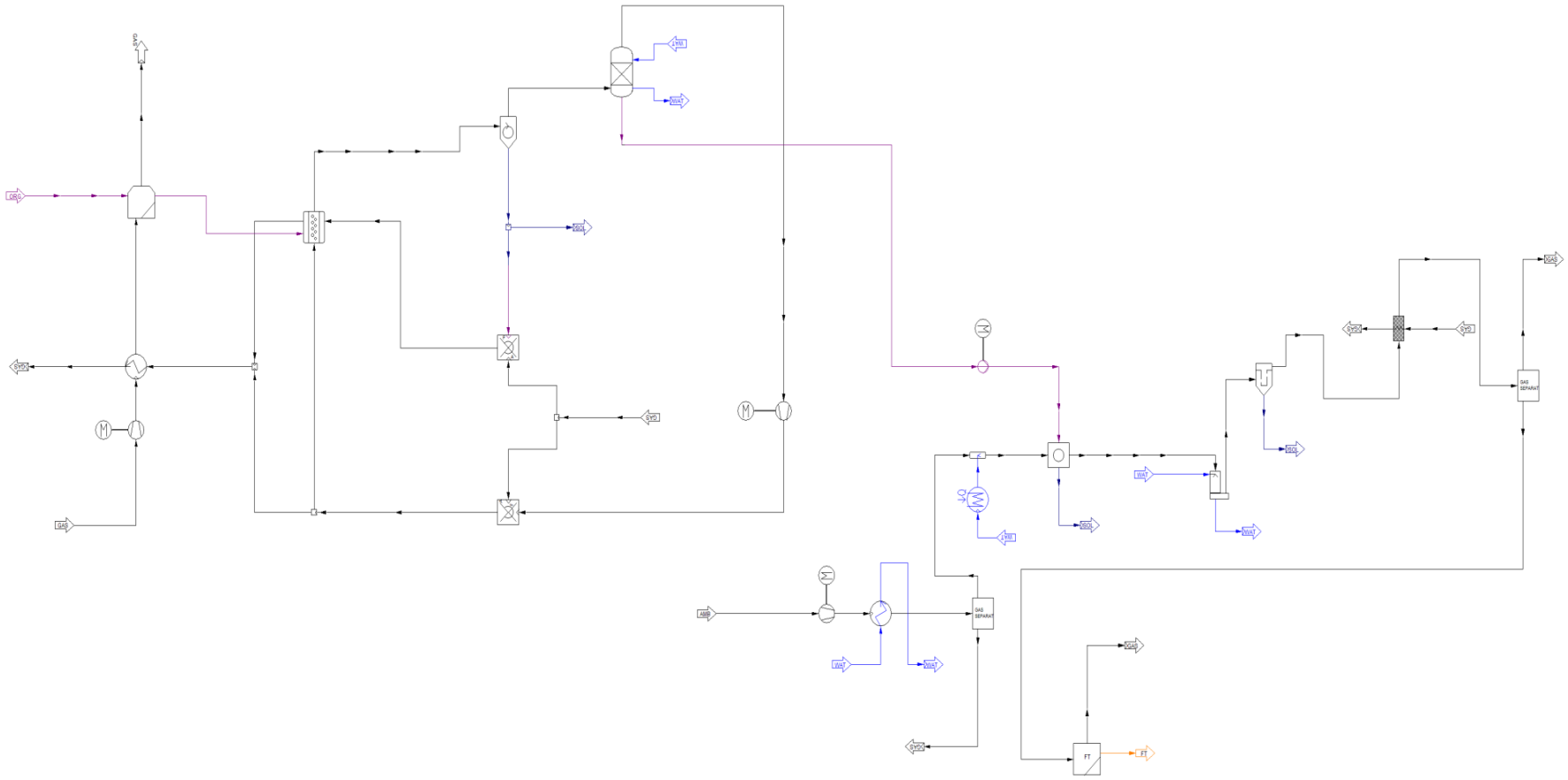

Figure 5-16: Flow sheet of the FP-FT process concept

The same was done for the other two fast pyrolysis based BTL concepts. The IPSEpro model of the fast pyrolysis process was given in section 5.5.5. This did not affect the simulation results of this study since the scale of the fast pyrolysis model can be increased (or decreased) according to the needs of the user. The gasification and gas cleaning steps were kept the same with the other entrained flow gasification based concepts. Table 5-26 shows the results of the simulation analysis of the FP-FT concept.

Table 5-26: Settings and results of the FP-FT concept simulation

Biomass		
LHV wet biomass	kJ/kg	13,056
Water content	%	30
Mass flow (wet)	kg/h	120,000
LHV daf biomass	kJ/kg	19,897
Mass flow (dry)	kg/h	84,000
Mass flow (dry)	t/d	2016
Bio-oil (as produced)		
LHV	kJ/kg	14,582
HHV	kJ/kg	16,284
Water content	%	27
Mass flow	kg/h	75,620
Mass flow	t/d	1815
FT-fuels		
LHV	kJ/kg	43,917
HHV	kJ/kg	47,276
Mass flow	kg/h	10,621
Mass flow	t/d	255
FT-off gas		
Mass flow	kg/h	30,175
Energy efficiency (eqn. 5-36)	%	28.2
FT-fuels mass yield (daf basis)	%	12.8

5.12.3.2 FP-MTG

Figure 5-17 shows the IPSEpro flowsheet of the FP-MTG concept. The only difference of the FP-MTG concept from the previous one is the fuels synthesis technology. The MTG

process was employed for this bio-oil gasification concept. Table 5-27 shows the results of the simulation of this concept on IPSEpro.

Table 5-27: Settings and results of the FP-MTG concept simulation

Biomass		
LHV wet biomass	kJ/kg	13,056
Water content	%	30
Mass flow (wet)	kg/h	120,000
LHV daf biomass	kJ/kg	19,896
Mass flow (dry)	kg/h	84,000
Mass flow (dry)	t/d	2016
Bio-oil (as produced)		
LHV	kJ/kg	14,582
HHV	kJ/kg	16,284
Water content	%	27
Mass flow	kg/h	75,620
Mass flow	t/d	1815
MTG-gasoline		
LHV	kJ/kg	42,301
HHV	kJ/kg	45,346
Mass flow	kg/h	9,465
Mass flow	t/d	227
MTG-off gas		
Mass flow	kg/h	13,978
Energy efficiency (eqn. 5-36)	%	24.2
Gasoline mass yield (daf basis)	%	11.4

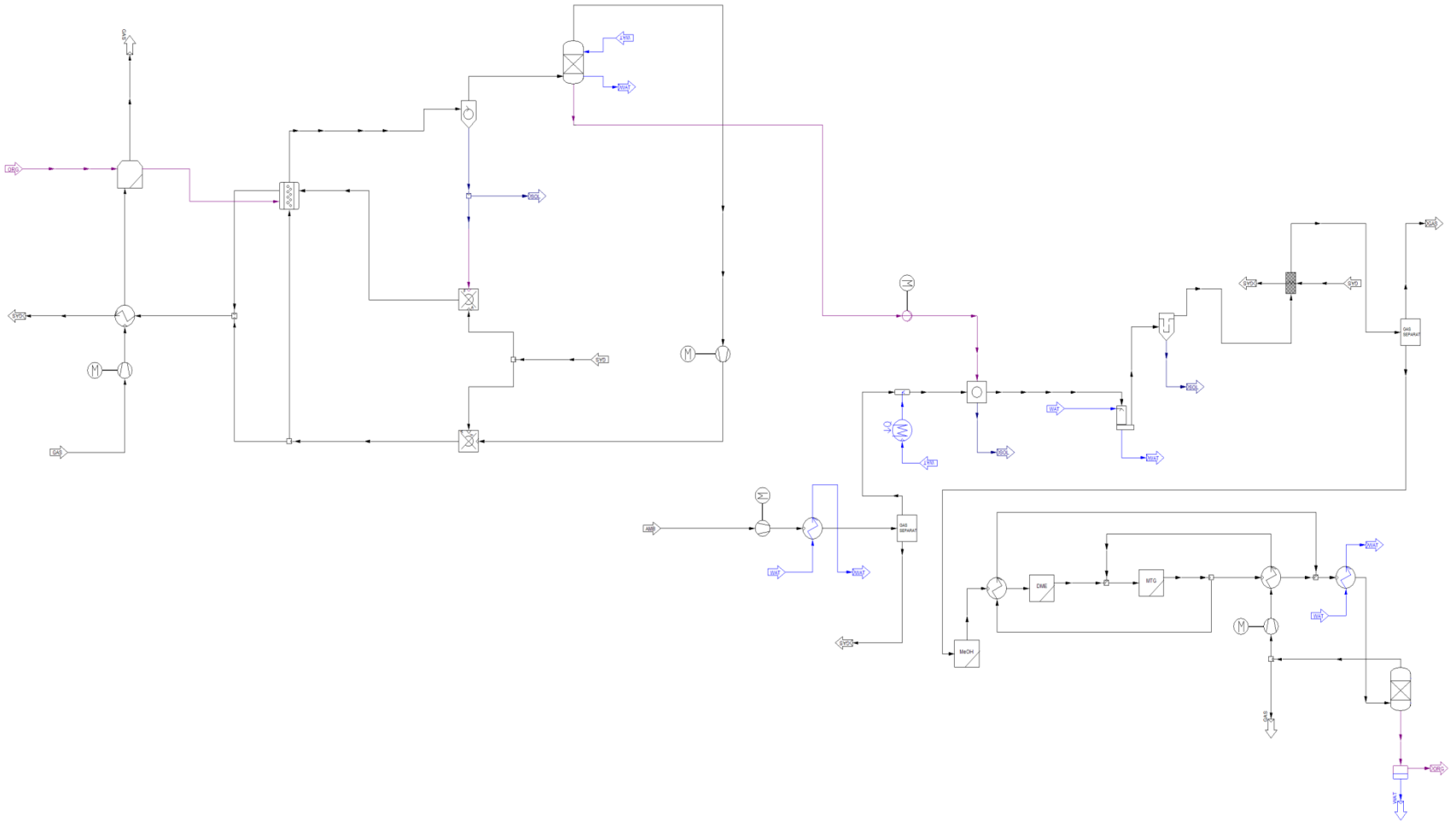

Figure 5-17: Flow sheet of the FP-MTG process concept

5.12.3.3 FP-TIG

The FP-TIG concept included entrained flow gasification and the TIGAS process as the fuel synthesis technology. The IPSEpro flow sheet of the concept is shown in Figure 5-18. The results of the simulation are shown in Table 5-28. It should be noted that the energy efficiencies of the all three BTL concepts based on bio-oil gasification are significantly lower the biomass gasification based BTL concepts. This was expected and it is further discussed in the next section.

Table 5-28: Settings and results of the FP-TIG concept simulation

Biomass		
LHV wet biomass	kJ/kg	13,056
Water content	%	30
Mass flow (wet)	kg/h	120,000
LHV daf biomass	kJ/kg	19,698
Mass flow (dry)	kg/h	84,000
Mass flow (dry)	t/d	2016
Bio-oil (as produced)		
LHV	kJ/kg	14,582
HHV	kJ/kg	16,284
Water content	%	27
Mass flow	kg/h	75,620
Mass flow	t/d	1815
MTG-gasoline		
LHV	kJ/kg	42,336
HHV	kJ/kg	45,381
Mass flow	kg/h	10,046
Mass flow	t/d	241.1
MTG-off gas		
Mass flow	kg/h	13,163
Energy efficiency (eqn. 5-36)	%	25.7
Gasoline mass yield (daf basis)	%	12.1

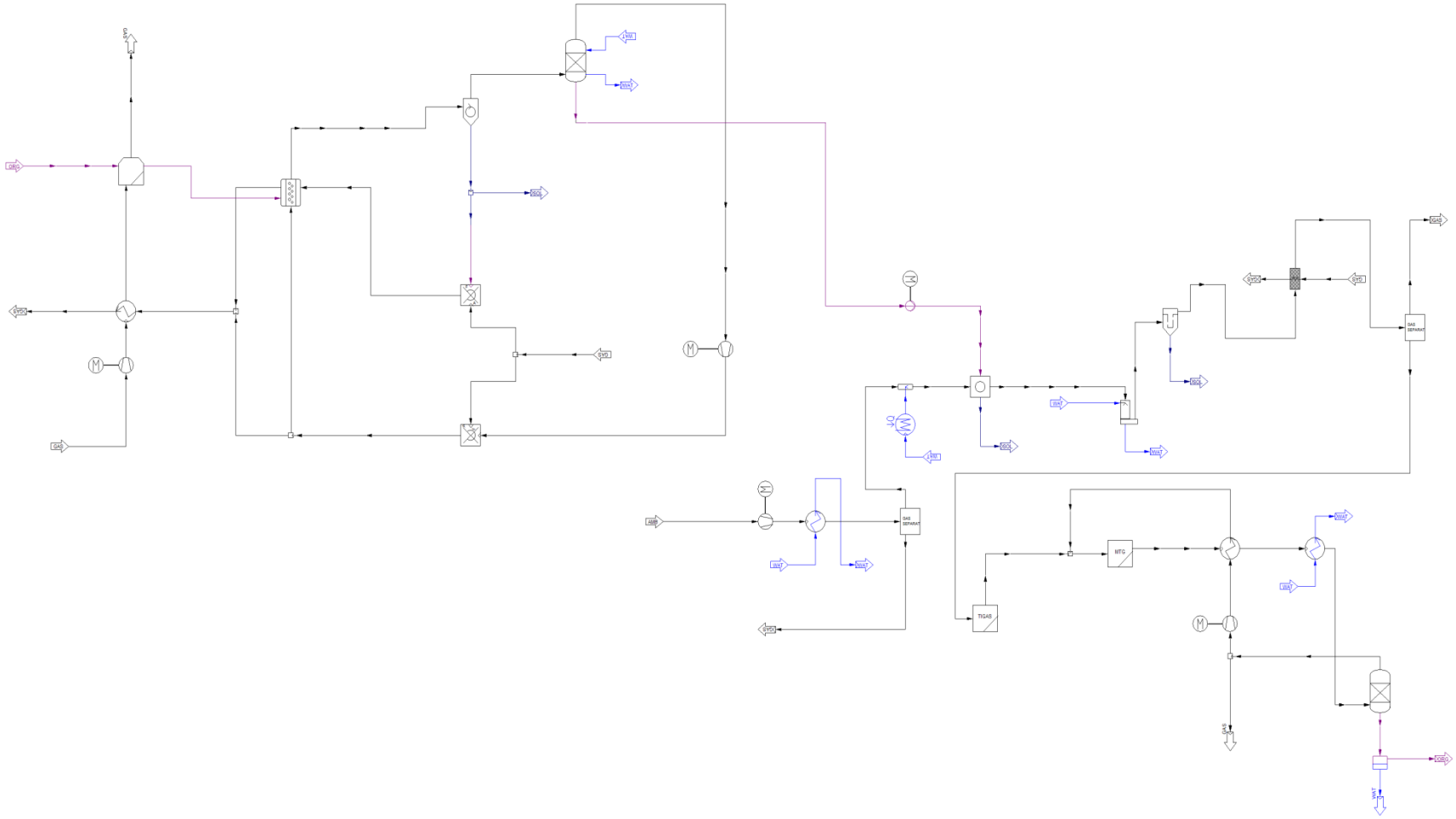

Figure 5-18: Flow sheet of the FP-TIG process concept

5.12.4 Concept comparison

The energy efficiencies of the nine BTL concepts evaluated in this study are summarised in Figure 5-19. Looking at the corresponding efficiencies shown in Figure 5-19, it becomes clear that the FT concepts perform better than the TIGAS and MTG concepts. Specifically, the CFB-FT concept shows the highest energy efficiency at 47.5%. This is due to the additional synthesis steps required in TIGAS and especially in the MTG process to produce liquid hydrocarbon fuels. The TIGAS process requires initially the synthesis of methanol and DME in the oxygenate synthesis reactor and then the synthesis of gasoline in another reactor (see section 5.11). The MTG process includes three subsequent synthesis steps: methanol synthesis, oxygenate synthesis and gasoline synthesis. As 100% conversion to the desired products is not achieved in any individual synthesis step, each additional synthesis step results in lower mass yields and thus lower energy conversion efficiencies.

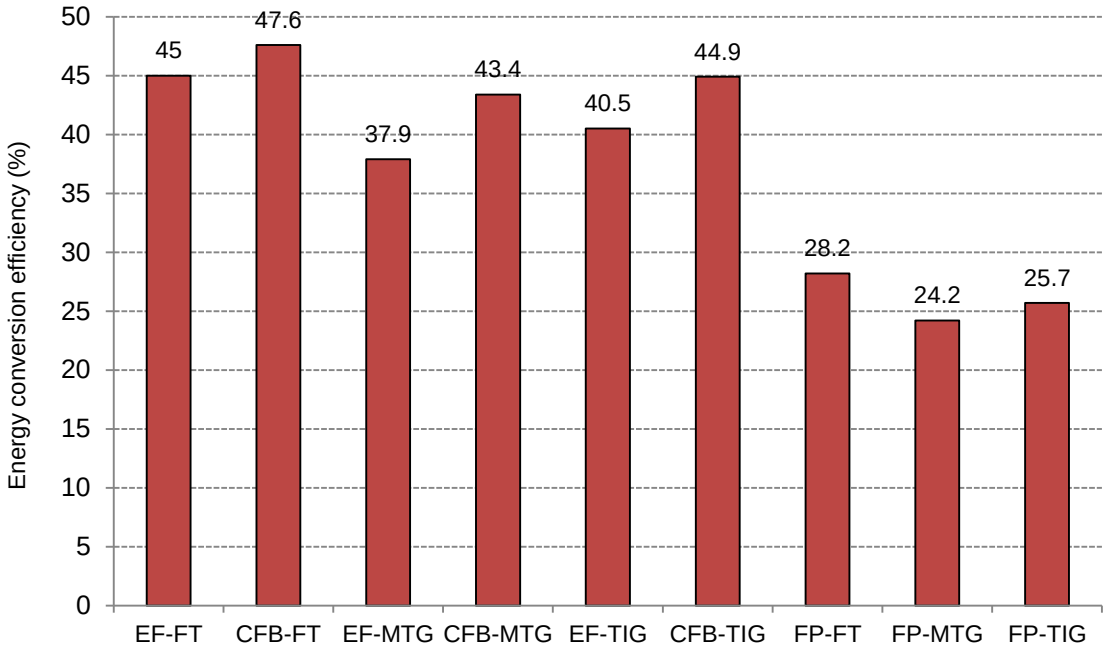

Figure 5-19: Energy conversion efficiencies (daf basis) of the evaluated BTL concepts

It can also be seen that CFB concepts deliver slightly higher energy conversion efficiencies by 2.6–5.5% than EF concepts with the same fuel production technology. This

is probably due to the loss of energy during quenching and cooling of the syngas after the entrained flow gasifier.

It also becomes clear that bio-oil gasification results in significantly lower energy efficiencies (by 14-17%) than direct gasification of biomass due to the additional thermal conversion step of fast pyrolysis. Fürnsinn [5] who, using IPSEpro, investigated the effect of biomass pre-treatment by fast pyrolysis on the plant's energy efficiency also reports lower energy efficiencies by 10-20% compared to direct biomass gasification. Based on these results, it seems questionable if decentralized pyrolysis pre-treatment with a centralized gasification and fuel synthesis plant could ever be competitive with direct gasification of biomass in terms of plant efficiency.

The mass yields of the nine BTL plant concepts are summarised in Figure 5-20. For the reasons discussed above FT synthesis performs better than the other fuel synthesis processes based on the same gasification technology. As expected, fast pyrolysis results in lower mass yields than the equivalent direct biomass gasification concepts.

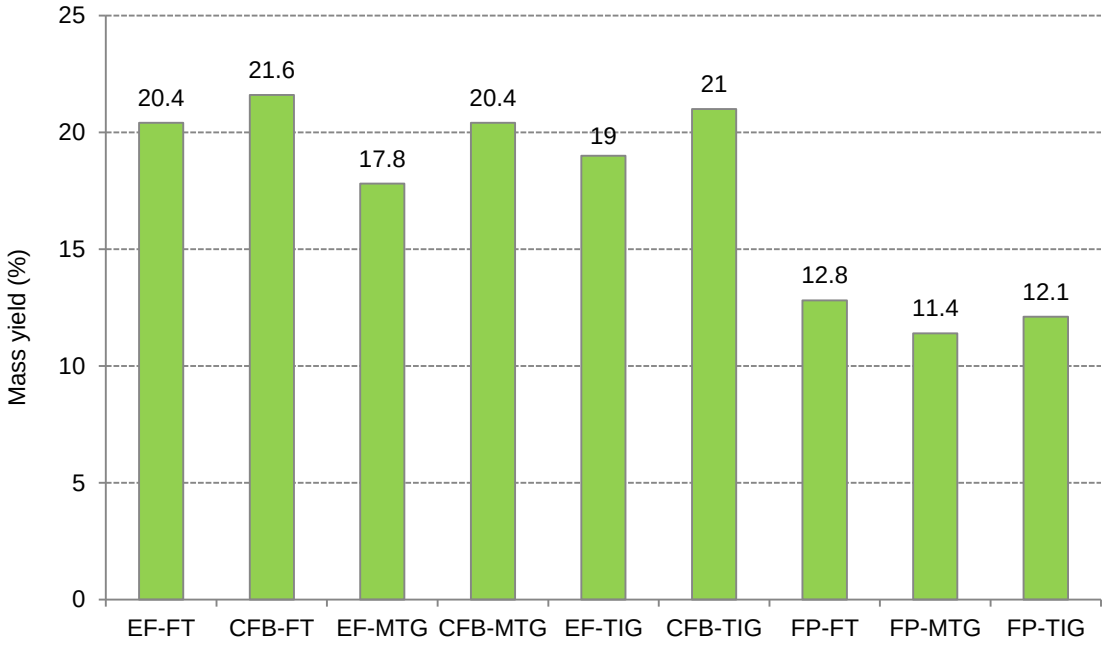

Figure 5-20: Mass yields (daf basis) of the evaluated BTL concepts

This study's results on the energy conversion efficiency of BTL plant concepts are consistent with those from other modelling studies (see Table 3-6 at section 3.3) which range from 36-55% (LHV). As a large-scale BTL plant has yet to be built the results of this study cannot be compared with a real industrial BTL plant. Bridgwater [12] reports that mass yields of BTL plants based on biomass gasification range from 14.9 to 23.5% on dry basis. The mass yield results of this study are well within this range.

6 ECONOMIC ASSESSMENT

6.1 Introduction

The previous chapters of this thesis have dealt with the description and the modelling of the technologies utilised for the thermo-chemical conversion of biomass to liquid hydrocarbon fuels. This chapter deals with the costs of these technologies and more specifically the costs of the nine BTL plant concepts evaluated in this study. One main purpose of the economic analysis is to identify the most promising BTL processes in terms of production costs. Another important aim is to examine whether BTL plants can compete economically with conventional transport fuels plants.

Firstly, a cost model was developed in MS Excel for each BTL concept to estimate capital, operating and production costs. A sensitivity analysis was then undertaken to investigate the effect of different cost parameters on the production costs of liquid fuels. Finally an uncertainty analysis was carried out to examine how the uncertainty in the input parameters of the cost model could affect the output (i.e. production cost) of the model.

6.2 General assumptions

6.2.1 Base year

The base year for the economic analysis was chosen to be 2009. This was the latest date for which US Chemical Engineering cost indices were available when the economic analysis study was started (late 2010). All cost data was therefore presented in 2009 GBP (£) using the Bank of England annual exchange rates [97]:

- 1 US ($) = 0.6389 GBP (£)
- 1 EUR (€) = 0.8911 GBP (£)

6.2.2 Plant life and operating hours

A plant life of 20 years was assumed, in line with the majority of similar techno-economic studies [90, 92, 94, 105, 107, 116]. A plant availability of 8,000 operating hours per year was used to account for maintenance downtime [12, 15, 88, 89, 94, 96].

6.3 Capital Costs

Capital costs are generally required in order to show the total amount of money necessary for the construction of an industrial plant. They also contribute to the estimation of production costs as will be discussed in section 6.4.1, therefore their calculation is necessary. The aim of this study is to calculate the *total plant cost* (TPC), which is the total investment needed to finance the project to the point at which the plant is ready to operate. The TPC, is also known as *fixed-capital investment* (FCI) [95, 98] and is an one-off cost thus it is not recovered at the end of the project life [98]. Conversely, the *working capital* (WC) which is the investment required to start the plant up, is recovered at the end of the project life [98, 99]. The sum of the fixed-capital investment and working capital is known as the *total capital investment* (TCI) [95, 98]. In this study the total capital investment was not used as a measure of capital cost since the working capital can be recovered at the end of the project life, thus the total plant cost was used instead.

The TPC of each modelled BTL concept was calculated using factorial estimation [95, 98]. This is an established cost estimation method reported by Peters [95] whereby the TPC is calculated from the total purchased equipment cost (TPEC) by using ratios based on cost breakdowns for a solid-fluid processing plant as shown in Table 6-1.

In order to estimate the TPC, each BTL plant concept was divided into plant modules in line with Brammer [165] and Toft [104]. The plant modules were the following:

- RSH and biomass preparation
- Biomass pre-treatment
- Gasification
- Gas cleaning and conditioning
- Fuel synthesis
- Refining
- Air separation
- Power generation

Firstly, the installed costs of all plant modules were estimated using reported costs from the literature. The installed costs are shown in Table 6-1 and include:

- Total purchased equipment cost (TPEC)

- Purchased equipment installation (PEI)
- Instrumentation and controls
- Piping
- Electrical systems
- Service facilities

Most literature costs used in this study were installed costs thus they included the costs mentioned above. In the rare case when a reported cost was not an installed cost, it was converted to an installed cost using the factors shown in Table 6-1. The installed cost of the plant was estimated as the sum of the installed costs of all plant modules.

Table 6-1: Calculation of total plant cost [95]

	%TPEC
Direct costs (installed)	
Total purchased equipment cost (TPEC)	100
Purchased equipment installation (PEI)	39
Instrumentation and controls	26
Piping	31
Electrical systems	10
Service facilities	55
Direct costs (non-installed)	
Buildings	29
Yard improvements	12
Land	6
Indirect costs	
Engineering and supervision	32
Construction expenses	34
Contractor's fee and legal expenses	23
Contingency	37
Total Plant Cost (TPC) = Direct + Indirect costs	

Table 6-2 shows the literature scales and installed costs which were used in this study for the estimation of the installed plant cost.

After the estimation of the installed plant cost, the TPEC was calculated using the estimated installed plant cost and the sum of the factors associated with all the installed direct costs (see Table 6-1):

$$\text{TPEC} = \text{Estimated installed plant cost} \times \frac{100}{261} \qquad (6\text{-}1)$$

This was done to estimate the remaining direct costs and the indirect costs from the TPEC using the respective factors shown in Table 6-1. The total plant cost was estimated as the sum of the installed direct costs, the non-installed direct costs and the indirect costs.

It is unusual to get a published cost estimate for the exact size of plant that is being considered. Thus the installed costs were scaled when necessary using the equation 3-1 in section 3.3. The Chemical Engineering Plant Cost Index was used to bring the cost to 2009 GBP (£) whenever a literature reported cost was from a previous year [95, 98]:

$$Cost\ in\ year\ 2009 = Cost\ in\ year\ B \cdot \frac{Cost\ index\ in\ year\ 2009}{Cost\ index\ in\ year\ B} \qquad (6\text{-}3)$$

The Chemical Engineering Plant Cost Index was used in this study as it was also used in the studies that the costs were taken from. Location factors were not applied to literature reported costs from different countries. This is mainly due to the lack of location data in much of the literature. Brennan [166] gives a spread of location factors among the US states (excluding Alaska and Hawaii) of 1.0 - 1.7 and a factor of 1.13 for the UK. Since most literature reported costs used in this study are from the US, it would appear reasonable to assume that average US and UK costs will be similar.

Table 6-2: Base scales and installed costs used in this study

Plant Module	Main items	Base capacity	Base cost (million US $)	Base year	Reference
RSH & preparation (EF)	Dryer, grinder	2000 dry t/d	21.3	2007	Swanson et al. [90]
RSH & preparation (CFB)	Dryer	2000 dry t/d	20.7	2007	Swanson et al. [90]
Fast pyrolysis - RSH & preparation[a]	Dryer, grinder	400 dry t/d	4.6	2006	Rogers [105]
Fast pyrolysis[b]	Fast pyrolysis reactor, Condenser	400 dry t/d	20.8 16.9 30.7	1995 2000 2008	Toft [104] Bridgwater et al. [167] Bridgwater [12]
Gasification & gas cleaning (EF)	EF gasifier, lockhopper, Water quench	2000 dry t/d	63.4	2007	Swanson et al. [90] Reed [168]
Gasification & gas cleaning (CFB)	CFB gasifier, lockhopper, tar cracker, syngas cooler	4536 dry t/d	112.9	2009	Larson et al. [114]
Gas conditioning (EF) - WGS	WGS reactor	1650 dry t/d	2	1991	Williams et al. [169]
Gas conditioning (EF & CFB) - Rectisol	Rectisol	1800 dry t/d 4536 dry t/d	14.5 44	1992 2009	WVU [170] Larson et al. [114]
Fuel synthesis (FT)	FT reactor	2000 dry t/d	42.2	2007	Swanson et al. [90]
Fuel synthesis (MeOH)	MeOH reactor	1650 dry t/d	38	1991	Williams et al. [169]
Fuel synthesis (MTG)	DME reactor MTG reactor	1735 t/d gasoline 1149 t/d gasoline	83.5 117	1982 1988	Grace et al. [171] Bridgwater et al. [172]
Fuel synthesis (TIGAS)	Oxygenate reactor MTG reactor	1735 t/d gasoline	44.5	1982	Grace et al. [171]
Refining (FT)	Hydrocracking	2000 dry t/d	42.2	2007	Swanson et al. [90]
Refining (MTG)	Included in the fuel synthesis cost				
Refining (TIGAS)	Included in the fuel synthesis cost				
Air separation		735 t/d O_2	24.3	2007	Swanson et al. [90]
Power generation	Steam turbine	14 % of other installed equipment costs [90, 92, 114]			

Notes to Table 6-2

(a),(b) The costs found in the literature for the fast pyrolysis process were total plant costs and thus apart from installed costs they also included other direct and indirect costs (see Table 6-1 for a full list of direct and indirect costs).

6.4 Production costs

Production costs on an annual basis are composed of operating costs, which typically include feedstock costs, raw materials costs, labour, utilities, maintenance and overheads, plus capital amortisation [95, 98]. Production costs are usually calculated on an annual basis since annual estimates smooth out the effect of any seasonal variations and provide a convenient way of considering large expenses that occur occasionally, such as annual planned maintenance shutdowns [95].

The production costs of transport hydrocarbon fuels were calculated on the basis of constant costs and performance for each year of operation of the plant [105, 107]. In most cases, plants (particularly those using new technologies) operate at reduced production rate during the first few years while the operators try to optimise the process [105]. Likewise, the operating costs tend to decrease with time as the operators become more experienced [105]. All biomass conversion technologies compared in this study are in a similar early stage of development so they have similar time profiles for performance and costs. Therefore, in order to make results comparable, the same assumption of constant costs and performance for each year of operation was used for all BTL concepts evaluated in this study. In reality, each year costs will increase in nominal terms because of inflation. However, revenues would also be expected to rise in nominal terms because of inflation and balance out the increase in costs. Therefore, it is considered reasonable to use real constant costs in this study provided that this is applied consistently. Additionally, inflation may well affect the operating costs, such as raw material prices, differently. Therefore, a decision between alternative BTL projects made without formally considering the effect of inflation on costs will still be correct, as inflation is likely to affect the cost estimates of all BTL concepts in a similar way [98]. In the following sections, the individual elements for the calculation of production costs are discussed.

6.4.1 Annual capital repayment

This cost calculation method amortizes the installed capital investment over the anticipated life of the plant at a given interest rate. The annual capital repayment is the money required to pay back the loan on capital which is required to set up the plant. It is calculated from the following equation [173]:

$$ACR = TPC \cdot \frac{r \cdot (1+r)^N}{(1+r)^N - 1} \qquad (6\text{-}4)$$

where ACR is the annual capital repayment, TPC the total plant cost, r the interest rate and N the plant life.

A reasonable interest rate has to be assumed in order to be able to apply this formula. RWE npower, a UK energy company involved in renewables including bio-energy, paid in 2009 a market (risk-free) interest of 4.5% [174]. If the annual capital repayment was calculated using a market interest rate, such as RWE's, the financial markets would have already taken inflation into account when setting the interest rate. As a result, an allowance for inflation would be built into the annual capital repayment but not into the other costs that comprise production costs. This problem can be overcome by removing the rate of inflation from the market interest rate, which is a nominal interest rate, and thus using the real interest rate. The Consumer Price Index (CPI), which is the measurement the UK governments use for inflation targets, reports an inflation rate of 2.2% for 2009 [175]. Therefore, the real interest rate that RWE paid in 2009 was approximately 2.3%. This real interest rate is considered very low for a new industrial BTL plant. It should be noted that the market interest rates as RWE's mentioned above, reflect the full range of businesses owned by energy companies. Many of these businesses are mature and are considered a low financial risk. It is likely that a new venture like a BTL plant would be considered high risk so it would be appropriate to use a higher interest rate. Consequently, a real interest rate of 10% was used in this thesis in line with similar techno-economic studies [16, 88, 105, 170].

6.4.2 Operating and maintenance costs

6.4.2.1 Fast pyrolysis

As discussed in section 4.4, biomass pre-treatment for the EF concepts based on bio-oil feed was done in five fast pyrolysis plants. O&M costs were estimated for each of the five fast pyrolysis plants and summed up to give the overall O&M cost of the biomass pre-treatment step.

Maintenance and overheads

Maintenance and fixed costs (insurance and taxes) were taken as 2.5% and 2% of the TPC respectively. This was in line with other techno-economic studies on fast pyrolysis [104, 105, 167].

Labour

Labour, as well as power requirements estimates were based on Rogers' study which provides a thorough and detailed comparison of staffing and power requirements of various fast pyrolysis studies.

Before estimating the number of plant employees, the number of shifts which an employee is likely to work in a year needed to be estimated first. This is shown in Table 6-3.

The wood chips RSH and preparation area was highly automated thus it was assumed that one operator was required for supervising the process. It was also assumed that the RSH and preparation area required staffing on a two shift basis (8 hours/shift) [105].

Table 6-3: Number of shifts worked by an employee in a year [105]

Rest days (2 days/week)	104
Holiday	25
Bank holiday	7
Sickness	9
Training	5
Total absence	150
Days/year	365
Shifts worked in a year	**215**

This was due to the fact that the biomass reception area is shut down at night with the drying process supervised by the plant operators at the pyrolysis area [105]. Reclaim and stock pile management were supervised by the front end loader driver [105]. The total staffing requirement for the RSH and preparation area of the fast pyrolysis plant is shown in Table 6-4.

Table 6-4: Labour requirement for the RSH and preparation area of the fast pyrolysis plant

Reception supervisors/shift	1
Shifts/day	2
Reception shifts/week	14
Front end loader drivers/shift	1
Shifts/day	2
Drivers shifts/week	14
Total shifts/week	28
Total shifts/year	**1456**
Shifts/employee/year (Table 6-3)	215
Employees required	**7**

The fast pyrolysis area was also assumed to be mostly automated but it also needed supervision. There has been insufficient operating experience to establish what the appropriate staffing requirement should be for a fast pyrolysis plant [105]. It would be reasonable to assume that the staffing structure would follow normal power station practice of having control room and plant operators [105]. The fast pyrolysis area would need staffing on a four shift basis, 2 persons per shift to cover health and safety requirements [12, 33, 167]. The total staffing requirement for the fast pyrolysis area is shown in Table 6-5.

Table 6-5: Labour requirement for the fast pyrolysis area

Shifts/day	4
shifts/week	28
Operators/shift	2
Total shifts/week	56
Total shifts/year	**2912**
Shifts/employee/year (Table 6-3)	215
Employees required	**14**

As shown in Table 6-4 and Table *6-5* the plant will require in total 21 employees. The cost per employee was assumed to be 41,000 $£_{2009}$/yr [105]. This rate was based on the average wage of employees in the energy and water sector plus payroll administration (5% of earnings) and employer's contribution to national insurance, staff pension and training [105].

Power requirements

According to Rogers, a 400 dry t/d fast pyrolysis plant requires an electrical consumption of 648 MJ/dry t (180 kWh/dry t) which corresponds to approximately 5180 GJ/yr (1.44 GWh/yr). The Department of Energy and Climate Change reports an average 2009 electricity price of 8.31p/kWh for large consumers [176]. This electricity price was used in this study to estimate costs from power consumption.

Heat requirements

Heat for the fast pyrolysis process is supplied by combustion of the char and off-gas as discussed in sections 4.4 and 5.5. While this simplifies the economic analysis, the system could be more cost-effective if the char was sold as a by-product (given that there was a market for it) and another energy source was used in the process. Future work would consider the various options available.

Bio-oil transport costs

Another important operating cost is the transportation cost of bio-oil to the central gasification plant. The costs associated with growing, harvesting storing and loading biomass into trucks are usually included in the biomass production costs. This is not the case for bio-oil so its transportation costs had to be estimated separately. It was assumed that bio-oil was transported to the central gasification plant by trucks in line with other similar studies [105, 167, 177]. Fixed and variable costs of bio-oil transportation costs were taken from two different literature sources shown in Table 6-6. The fixed cost includes the loading and unloading cost of bio-oil between trucks and storage tank [177]. The variable cost of bio-oil transportation by truck includes fuel consumed by engine, labour and maintenance charges [177]. Both studies gave similar results therefore the bio-oil transportation cost was taken as the average of the reported costs.

Table 6-6: Bio-oil transportation costs used in this study

Reference	Truck capacity	Base date	Fixed cost	Variable cost
Pootakham [177]	30 m^3	2010	5.67 \$/m^3	0.07 \$/m^3/km
Bridgwater [167]	30.5 tonnes	2000	4.29 €/t	0.039 €/t/km

A full analysis of transport distances can only be performed on a case by case basis, taking account of actual bio-oil production areas, local topography, the road network and

other case-specific features. This study requires a more generic approach and the following assumptions were made:

1. Bio-oil production is evenly distributed over a circular bio-oil supply area. The central gasification plant is in the middle of this area.
2. Each fast pyrolysis plant is identical.
3. The road network to the central gasification plant is regular and symmetrical.
4. The distance between the central gasification plant and a fast pyrolysis plant is maximum 100 km [177].

6.4.2.2 Gasification and fuel synthesis plant

There appears to be limited consensus in the literature as to the staffing level as well as utilities costs and requirements for large-scale BTL plants. To deal with this problem operating costs can be taken instead as a percentage of the fixed capital investment. Van Vliet et al. [88] assumed that the O&M costs (labour, maintenance, raw materials, waste disposal, utilities) were 4% of the fixed capital investment. These costs did not include power requirements and fixed costs (insurance, taxes). Hamelinck et al. [62], as well as Larson et al. [114] made the same assumption (4% TPC) for the O&M costs of large-scale BTL plants. Swanson et al. [90], whose study was reviewed in Chapter 3 (section 3.2.4), give detailed capital and operating costs of BTL plants. In their study, operating costs including fixed costs were approximately 6% of the fixed capital investment. Fixed costs are usually taken as a percentage of the fixed capital, which is assumed to be 1.5-2% [95, 98]. Therefore, Swanson's results are in accordance with the other studies. Bridgwater also reported that the materials, utilities and labour costs of large scale BTL plants are approximately 2.2% of the fixed capital investment [12]. By assuming a maintenance cost of 2.5% of TPC [33, 167], Bridgwater's reported O&M cost is 4.7% of TPC [12]. Therefore, in this study, O&M costs of the gasification and fuel synthesis plant were assumed to be 5% of the TPC. Adding the fixed costs, which were assumed to be 2% of the TPC [95, 98], the total operating costs were 7% of the TPC.

6.4.3 Biomass costs

Wood chips cost estimates were based on Rogers' study [105] who provides a comprehensive and thorough study on wood chips production costs. The price of wood chips was 54.41 $£_{2006}$/dry t and this included growing, harvesting and storage, as well as

transporting biomass to the gasification plant [105]. This biomass cost reported by Rogers was adjusted to 58.6 £$_{2009}$/dry t using a 2.5% inflation rate from the Bank of England's web site [97].The cost of biomass can vary significantly and it mainly depends on the biomass yield and the land available for cultivation [105]. The biomass feedstock cost is an important element of the production cost [12] and thus its effect was investigated in the sensitivity and uncertainty analysis sections (section 6.6 and 6.7, respectively).

6.5 Results

This section presents and evaluates the capital and production costs results of the nine BTL plant concepts. A comparison between all modelled BTL concepts for processing 2016 dry t biomass per day is made based on their capital and production costs. The results are then compared to the production costs of conventional transport fuel plants. The estimated capital, operating and production costs for each concept are presented in detail in Appendix C. The nine BTL concepts are summarised in Table 6-7 from Table 4-1 in section 4.9.

Table 6-7: The nine BTL concepts evaluated in this study

BTL concept	Pre-treatment	Gasification	Fuel synthesis	Product
EF-FT		EF	FT	Diesel, Gasoline, Kerosene
EF-MTG		EF	MTG	Gasoline
EF-TIG		EF	TIGAS	Gasoline
CFB-FT		CFB	FT	Diesel, Gasoline, Kerosene
CFB-MTG		CFB	MTG	Gasoline
CFB-TIG		CFB	TIGAS	Gasoline
FP-FT	Fast pyrolysis	EF	FT	Diesel, Gasoline, Kerosene
FP-MTG	Fast pyrolysis	EF	MTG	Gasoline
FP-TIG	Fast pyrolysis	EF	TIGAS	Gasoline

6.5.1 Capital costs

Figure 6-1 shows the breakdown of capital costs by area and resulting total plant cost for all nine BTL plant concepts summarised in Table 6-7 above. As discussed in section 6.2.1, the base year for the economic assessment study was 2009 and the costs were presented in British Pounds. The total plant cost data used for Figure 6-1 is shown in Table 6-8.

It can be seen that the estimated capital costs of large-scale BTL plants range from 264 to 390 million GBP. All the MTG based concepts give higher capital costs by up to 27% than the equivalent FT and TIGAS based concepts.

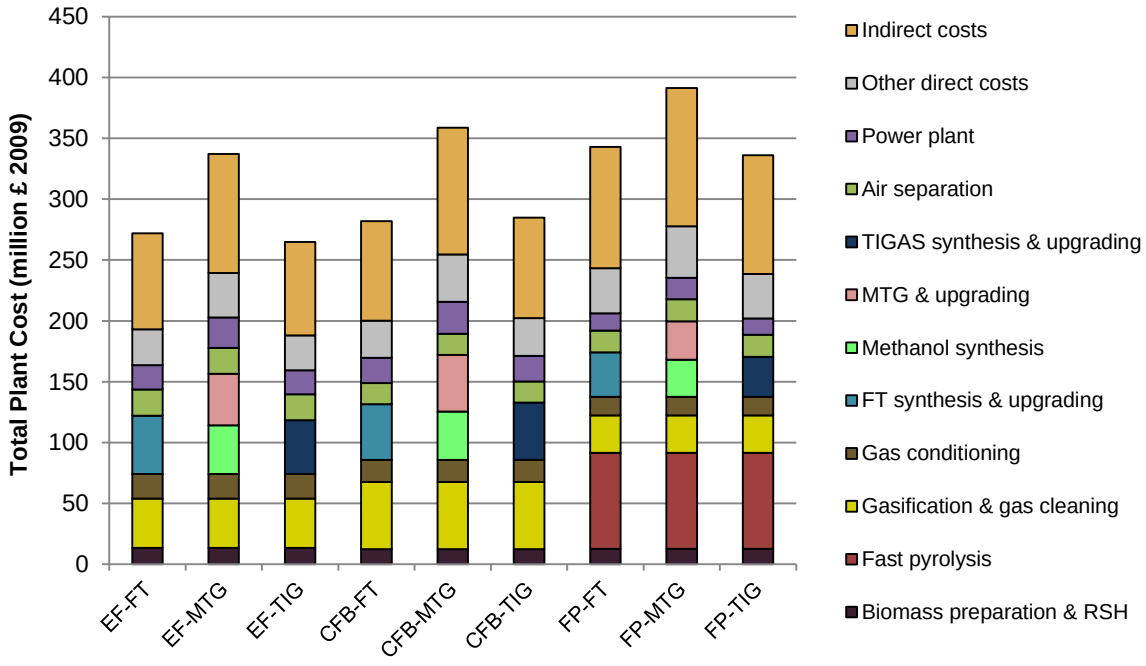

Figure 6-1: Total plant costs of the evaluated BTL concepts (2016 dry t/d)

This difference is easy to understand since the MTG process includes the additional conversion step of methanol synthesis. A significant portion of methanol synthesis capital cost is the syngas compression to 50 bar which is the operating pressure of methanol synthesis. According to Swanson et al. [90], compressors have high purchase costs and can make up of approximately 18% of the purchased equipment costs of BTL plants. The additional compression step required for the MTG process would result in higher compression equipment requirements than the FT and TIGAS concepts and thus will significantly increase the capital cost of the MTG process.

Table 6-8: Breakdown of total plant costs (million £$_{2009}$) of the nine BTL concepts evaluated in this study

	EF-FT	EF-MTG	EF-TIG	CFB-FT	CFB-MTG	CFB-TIG	FP-FT	FP-MTG	FP-TIG
Biomass preparation & RSH	13.60	13.60	13.60	12.34	12.34	12.34	12.58	12.58	12.58
Fast pyrolysis	-	-	-	-	-	-	78.89	78.89	78.89
Gasification & gas cleaning	40.45	40.45	40.45	55.28	55.28	55.28	30.79	30.79	30.79
Gas conditioning	20.14	20.14	20.14	18.04	18.04	18.04	15.33	15.33	15.33
FT synthesis & upgrading	47.97	-	-	45.75	-	-	36.51	-	-
Methanol synthesis	-	39.95	-	-	39.95	-	-	30.41	-
MTG & upgrading	-	42.34	-	-	46.28	-	-	31.65	-
TIGAS synthesis & upgrading	-	-	44.22	-	-	47.27	-	-	32.90
Air separation	21.36	21.36	21.36	17.35	17.35	17.35	18.01	18.01	18.01
Power plant	20.09	24.90	19.57	20.83	26.49	21.04	14.09	17.67	13.58
Other direct costs	29.46	36.51	28.69	30.54	38.85	30.85	37.13	42.38	36.40
Indirect costs	78.98	97.87	76.92	81.87	104.15	82.70	99.54	113.60	97.56
TOTAL	272.05	337.11	264.94	281.98	358.72	284.87	342.86	391.29	336.02

The major process areas of capital investment for all BTL concepts based on solid biomass gasification, are the gasification and gas clean-up area and the fuel synthesis area. This is in line with all techno-economic studies of BTL plants reviewed in Chapter 3. The BTL concepts based on the CFB gasification technology have higher gasification and gas clean up costs than the EF based concepts due to the need for a tar cracker and the additional heat exchange equipment required for syngas cooling. As discussed in section 4.6, syngas cooling for the EF concepts was done by a water quench thus a heat exchanger was not employed.

Figure 6-1 also shows that in general bio-oil gasification results in higher capital costs than solid biomass gasification. Even though the gasification plant of the bio-oil gasification concepts is smaller than this of the solid biomass gasification concepts the overall capital costs are higher. This was due to additional process step of fast pyrolysis which makes up of approximately 20-24 % of the TPC of the bio-oil gasification concepts. Nevertheless, it is interesting to see that the FP-TIG concept results in lower capital costs than the EF-MTG and the CFB-MTG concepts, although the FP-TIG concept employs a different fuel synthesis technology (TIGAS) than the other two concepts (MTG).

This study's results on the capital costs of BTL plant concepts are consistent with those from similar modelling studies of the same gasification technologies which range from 238-552 million GBP_{2009} (see Table 3-6 at section 3.3). However, cost comparisons with other studies should be made with caution due to the different financing assumptions of each study. For example, Swanson et al. [90] assumed a 15% working capital as an additional cost to his capital investment. Additionally, Jones et al. [94] and Philips et al. [92] assumed a 5% working capital of fixed capital investment. As discussed in section 6.3, this study did not consider working capital since this can be recovered at the end of the project. Therefore, if working capital was removed from the capital cost estimations of these three studies, their reported capital costs would be lower.

6.5.2 Operating and maintenance costs (O&M)

Figure 6-2 shows the annual operating and maintenance costs which included biomass costs and capital dependent operating costs (see section 6.4.2). It is clear that biomass cost is the largest contributor to O&M costs and represents essentially more than 50% of the annual O&M costs for all BTL concepts. Once again the MTG concepts have higher

costs than the FT and TIGAS concepts. This was expected since most O&M costs are a fraction of the TPC as explained in section 6.4.2.

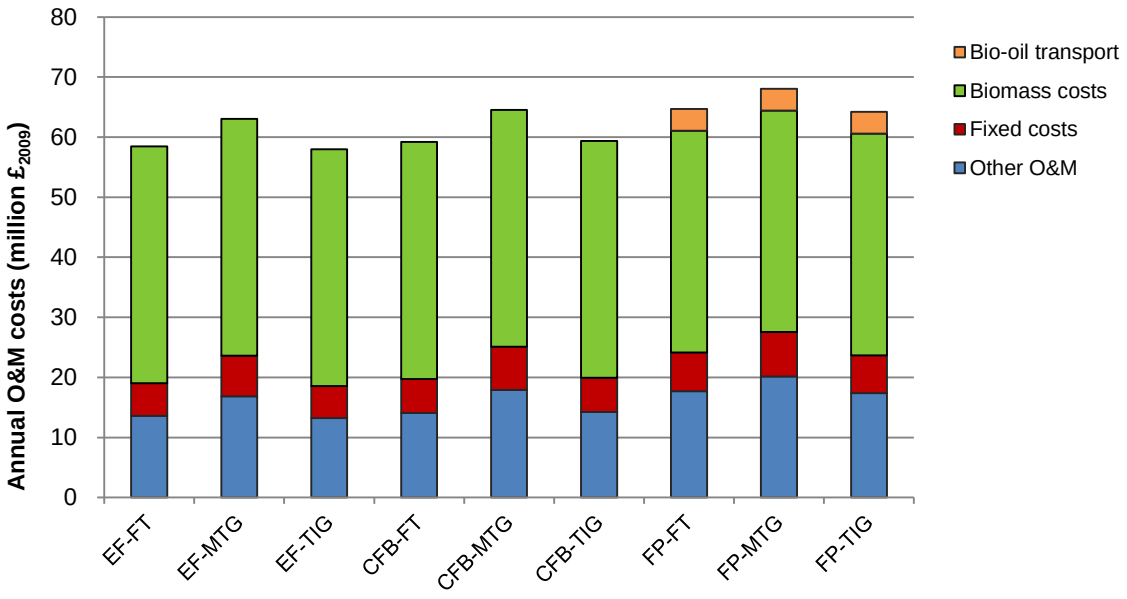

Figure 6-2: Annual operating and maintenance costs of the evaluated BTL concepts

There is confusing Information on O&M costs in the literature. Annual O&M costs are usually not reported at all in other studies and if provided are expressed in $/gal, $/t or $/GJ of product. According to Swanson et al. (reviewed in section 3.2.4), O&M costs of large-scale BTL plants based on FT synthesis are approximately 50 million GBP_{2009} [90]. Hamelinck et al., whose study was reviewed in section 3.2.1, reports similar O&M costs of approximately 42 million GBP_{2009} [15]. The estimated O&M costs of the FT-concepts of this study are higher than those of Swanson and Hamelinck. However both studies used lower feedstock prices than this study, therefore this study resulted in higher O&M costs compared to those of Swanson and Hamelinck. Jones et al., whose study was reviewed in section 3.2.5, studied the costs and performance of fixed bed MTG plants [94]. His reported O&M costs were approximately 37 million GBP_{2009} and thus lower than the other two studies [94]. However, Jones's results need to be looked at with scepticism since MTG based BTL plants should result to higher O&M than FT synthesis based plants of the same scale due to the cost penalty associated with the additional process step of methanol synthesis.

6.5.3 Production costs

6.5.3.1 Concept comparison

Figure 6-3 shows the estimated production costs of all BTL plant concepts evaluated in this study. This includes a comparison with the average tax free market price of conventional transport fuels at the refinery gate in 2009.

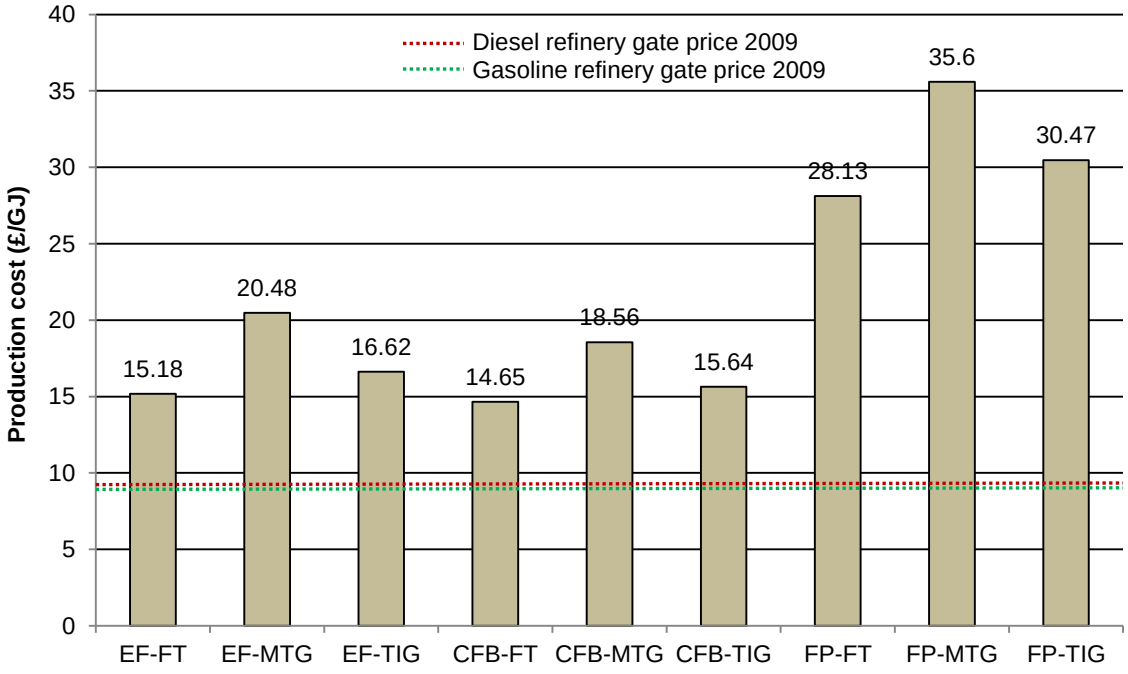

Figure 6-3: Production costs of the evaluated BTL concepts in £$_{2009}$/GJ (LHV)

It can be seen that the BTL plants based on FT synthesis result in lower production costs than the TIGAS and MTG based BTL plants. More specifically, the CFB-FT concept gives the lowest production costs of liquid hydrocarbon fuels at 14.65 £/GJ. It is closely followed by the EF-FT concept at 15.18 £/GJ. Even though the EF-FT concept results in lower capital and O&M costs than the CFB-FT concept (see section 6.5.1 and 6.5.2), the latter gives lower production costs due to the slightly higher efficiency of the CFB-FT concept for the reasons explained in section 5.12.4. From this it is clear that efficiency (and thus production rate) is a very important element of the production costs thus its effect was investigated in the sensitivity and uncertainty analysis sections (section 6.6 and 6.7, respectively).

TIGAS is the second most economic fuel synthesis option after FT synthesis. As discussed in section 5.12.4 and 6.5.1, TIGAS based concepts resulted in lower energy efficiencies and higher costs since the TIGAS process is more complex than FT synthesis. Therefore, the TIGAS concepts give higher production costs than the FT synthesis concepts.

The BTL concepts based on the MTG process always result in higher production costs than the FT and TIGAS based concepts due to the increased complexity associated with the inclusion of the methanol synthesis process and the lower efficiencies (see section 5.12.4). The EF-MTG concept gives the highest production cost among all the biomass gasification concepts at 20.48 £/GJ.

Bio-oil gasification for biofuel production is much more expensive than solid biomass gasification as shown in Figure 6-3. Although capital and operating costs are slightly higher than the equivalent solid biomass concepts, the conversion efficiency is much lower thus leading to much higher production costs. Therefore, it seems questionable if fast pyrolysis coupled with gasification will ever be an economically viable option for the production of liquid hydrocarbon fuels.

Figure 6-4 shows the contribution of capital costs, O&M costs including fixed costs and biomass costs to the estimated production costs of liquid hydrocarbon fuels. It can be seen that biomass cost is a very important contributor to the production costs as it represents approximately 43-44% of the overall production costs of the solid biomass gasification concepts. Therefore, its effect will be examined in the sensitivity and uncertainty analysis sections. Capital costs have also a significant effect representing approximately 35-40% of the production costs of the biomass gasification concepts. Capital costs are slightly more important for the bio-oil gasification concepts than the biomass gasification concepts as they represent approximately 38-40% of the production costs. This shows the impact that the additional process step of fast pyrolysis has on the overall BTL process costs.

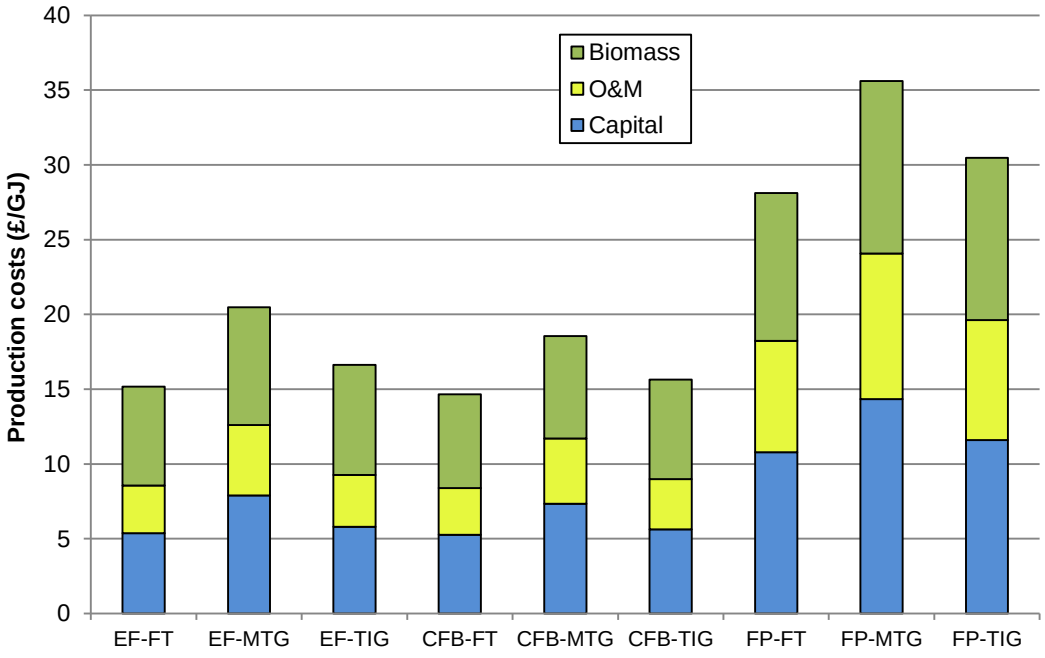

Figure 6-4: Production costs breakdown

This study's results on the production costs of BTL plant concepts are consistent with those from similar modelling studies of the same scale and same gasification technologies which range from 11.8-20.8 £/GJ (see Table 3-6 at section 3.3).

6.5.3.2 Comparison with market price of fossil transport fuels

Figure 6-3 also provides a comparison between the BTL production costs and the 2009 price of fossil diesel and gasoline. The 2009 refinery gate (tax-free) prices of conventional diesel and gasoline were 8.8 £/GJ and 8.6 £/GJ, respectively and were taken from the UK petroleum industry association (UKPIA) website [178]. The fuel prices reported in the UKPIA website are given in £/l. These were converted to £/GJ by using a volumetric energy density of 34 MJ/l (LHV) and 32 MJ/l (LHV) for diesel and gasoline, respectively [100].

The aforementioned refinery gate prices of conventional diesel and gasoline do not include taxes, profit for the producer and retailer, marketing and distribution costs so that a comparison can be made with the estimated biofuel costs of this study. As such, they are not the retail prices (also known as pump prices) that the consumer would pay at the petrol

station. The fuel retail prices for the same year were 31.2 £/GJ for gasoline and 30.6 £/GJ for diesel [178]. It can be seen that the prices of diesel and gasoline are very similar. The refinery gate price of jet fuel (kerosene), which is produced from FT synthesis, is not reported in the UKPIA website and could not be found elsewhere. A comparison of transport fuels retail prices is available on the Index Mundi website [179]. From this it is clear that the retail prices of diesel, gasoline and kerosene in 2009 were very similar. Therefore, it would appear reasonable to assume that the refinery gate price of kerosene in 2009 would also be similar to the refinery gate prices of diesel and gasoline shown in Figure 6-3.

Figure 6-3 shows that BTL plants cannot compete with the costs of the large conventional fuel production plants. It would require increases in fossil fuel prices, subsidies or legislation such as high carbon taxes to make 2nd generation transport biofuels competitive in the market. It can be seen that the CFB-FT concept (the main product is diesel) is closer than the other concepts to matching the reference diesel price which is approximately 65% lower. The other concepts will require further development to reduce costs before they can be economic but viability by this route is a likely prospect. In the case of gasoline, the CFB-TIG concept results in a biomass derived gasoline price of approximately 82% higher than the reference gasoline price.

Nevertheless, based on the constantly increasing fossil fuels prices and the current subsidies for bioenergy applications, BTL production is considered promising. More specifically, the current retail diesel and gasoline price is 41.3 £/GJ and 42.4 £/GJ [180], thus higher than the 2009 prices. In addition, through the Renewables Obligation (RO), the UK government already makes generous subsidies available for biomass-based electricity production. The RO requires licensed UK electricity suppliers to derive from renewable sources a specified and annually increasing proportion of electricity they supply to customers, or pay a penalty [181]. Such subsidy schemes are driven by a combination of the pressures described in Chapter 1. According to the Wood Panel Industries Federation (WPIF), these UK subsidies amount to £75 per tonne of wood burned in a power plant [182]. A co-firing station, which is a plant that burns biomass alongside coal, receives about £25-£50/t of wood burned [182].

For the CFB-FT concept, which was the most economic BTL system, a subsidy of approximately £55/t of dried wood would be required to meet the conventional fuel prices shown in Figure 6-3. The necessary biomass subsidy was estimated by iterating the cost model of the CFB-FT concept to get the conventional fuel price (8.7 £/GJ on average). If the £75/t subsidy reported by the WPIF was used instead, the production costs of the CFB-FT concept will significantly reduced by almost half of the estimated costs. However, these promotional measures are usually aimed at small or medium-sized power plants and it is therefore questionable if they can be applied for large scale BTL installations. Many government programmes have limited budget or are tied to certain technologies, thus a project of this size might not be subsidised. Government subsidies would mainly depend on the political climate and thus their level is still unknown. Furthermore, subsidies of this kind have other consequences such as the increase in biomass costs. For example, since 2005, the price of wood used in the construction and wood panel industries has risen by more than 50% in the UK as a result of the aforementioned biomass subsidies which have increased demand for wood [182].

Apart from biomass subsidies, there are also other subsidies associated with capital investment (e.g. Enhanced Capital Allowance (ECA) scheme [183]), government taxes and biofuel products (e.g. RTFC). With regards to transport biofuels subsidies, according to the Renewable Transport Fuels Obligation (RTFO), which was also discussed in section 1.1, UK owners of biofuels are awarded one Renewable Transport Fuel Certificate (RTFC) per litre of biofuel, or kilogram of biomethane, supplied [184]. The value of the RTFC is not fixed as it depends on the market [184]. Biofuels produced from certain feedstocks are eligible for double counting [184]. These include biofuels derived from wastes and residues as well as those from non-edible ligno-cellulosic biomass [184]. RTFCs may be traded between participants in the scheme thus even the smallest biofuel company may claim certificates which can potentially be sold to obligated fuel producers that may then use them to meet their 5% obligation.

It should be noted that in July 2012, the Department of Energy and Climate Change (DECC) announced that it will continue to subsidise bioenergy applications under the Renewable Obligation Certification scheme [185]. There is however the possibility that public and political support for subsidising bioenergy could wane due to lack of interest and budget restrictions. Although such schemes are valuable opportunities for BTL plants

in the short term, it would be far better to find markets (e.g. chemicals) that could be penetrated without any subsidies.

6.6 Sensitivity analysis

The evaluations thus far have taken the results of the models at face value, therefore sensitivities and uncertainties in the models have not been considered yet. This section discusses the sensitivity analysis study which was conducted in order to investigate the effect of parameters variations on the production costs results.

In the previous section some parameters were identified as having an important effect on the production costs of liquid hydrocarbon fuels. These parameters were selected for the sensitivity analysis and were: biofuels production rate (GJ/h), capital costs (i.e. TPC) and biomass cost. Other parameters included: O&M costs, real interest rate, plant availability and plant life as these were identified by other studies for also significantly affecting production costs [90, 104, 167]. The sensitivity analysis was carried out by changing each parameter in turn by ±10% of its default value. It should be noted that the plant availability parameter (see section 6.2.2) was changed by -10% to +5% since the plant's operating hours cannot exceed the maximum hours per year (+110% of 8000hrs/yr = 8800>8760 hrs). The sensitivity analysis results of the CFB-FT concept, which was the most economic BTL system, are presented here. The sensitivity analysis of the other BTL concepts gave similar results with the CFB-FT concept thus the sensitivity analysis results of the other BTL concepts are presented in Appendix C.

Figure 6-5 shows the sensitivity of the production costs of the CFB-FT concept to the variations of the selected model parameters. Figure 6-5 is a spider plot which is widely used for presenting sensitivity analysis results. Steeper curves indicate a higher degree of sensitivity to deviations from the original estimates/values of the model parameters. The point in the graph where all lines meet indicates the original estimated value of the cost model's output (i.e. biofuel production cost).

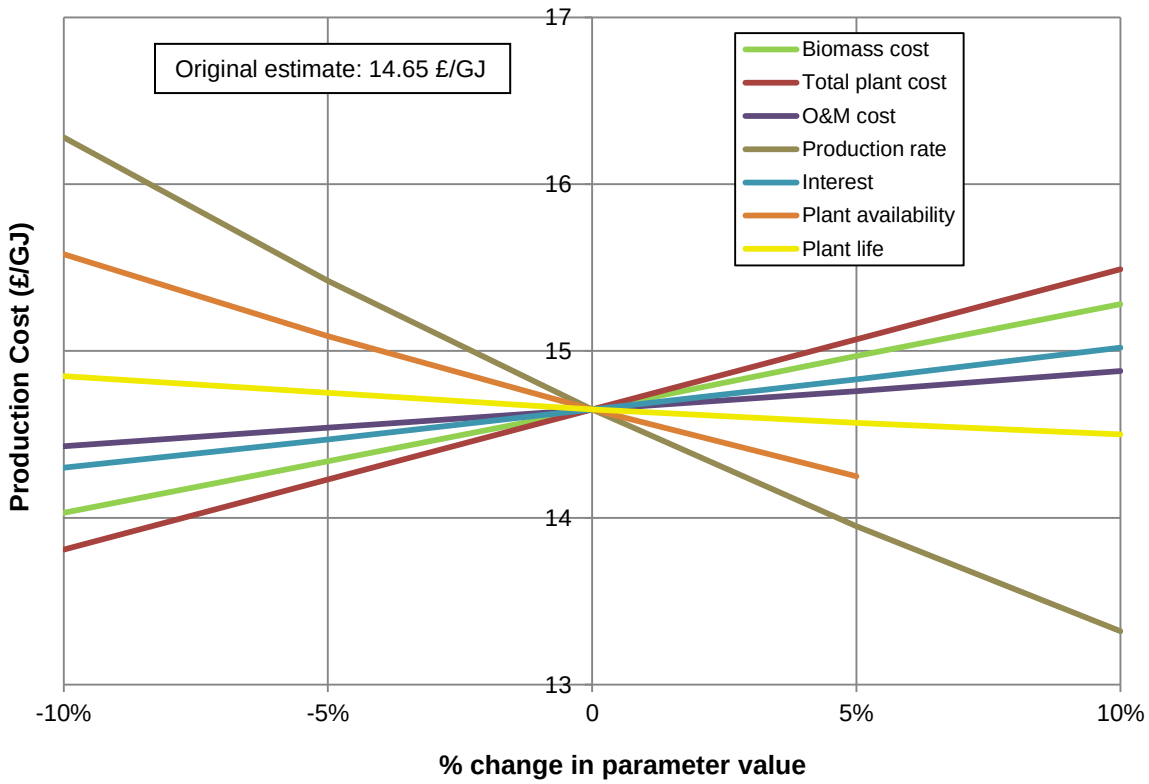

Figure 6-5: Sensitivity of biofuel production cost of the CFB-FT concept

Table 6-9 shows the variations on production costs of the CFB-FT concept which resulted from the variations of the selected model parameters from their default value. From Figure 6-5 and Table 6-9 it can be seen that production rate is the most sensitive model parameter which has the greatest effect on production costs. The product energy yield used as a default (47.6%) is a reasonable estimate of the IPSEpro model since the vast majority of published studies on techno-economics of large-scale BTL plants based on FT synthesis report energy yields of 39-50% (see Table 3-6 at section 3.3). The performance of FT synthesis reactors in general is established but there is limited experience of FT reactors operation using biomass derived syngas. This increases the uncertainty of the overall results. The sensitivity of the model to the production rate of biofuels suggests that improving process performance should be an early priority.

Table 6-9: Production costs of the CFB-FT concept as a result of parameters' variations

	-10%	-5%	0	5%	10%
Biomass cost	14.03	14.34	14.65	14.97	15.28
Total plant cost	13.81	14.23	14.65	15.07	15.49
O&M cost	14.43	14.54	14.65	14.76	14.88
Production rate	16.28	15.42	14.65	13.95	13.32
Interest	14.3	14.47	14.65	14.83	15.02
Plant availability	15.58	15.09	14.65	14.25	-
Plant life	14.85	14.75	14.65	14.57	14.5

The plant availability is the next most sensitive parameter. Therefore, it is imperative to the viability of large scale BTL plants that the plant operating hours are as high as possible to maximise annual production and reduce production costs. The 8000 hrs/yr default availability which was selected in the model is a reasonable estimate, however situations can occur, such as seasonal demand or feedstock availability, where this parameter must be carefully set to prevent serious errors in the calculated biofuel production costs. The experience gained in the first year of the plant's operation and the optimisation carried out in the meantime will most likely result in an increase in the plant availability.

The plant availability is closely followed by the overall total plant cost with regards to the impact on production costs. Regarding the calculated value, there is some uncertainty inevitable in study estimates of this type. Errors of ±30% are typical, and increased accuracy can only be achieved through very detailed and expensive analysis of the specific case study. It should be noted that there are inherent uncertainties in projecting BTL plant costs given the pre-commercial status of some of the major pieces of equipment included in the concepts examined. The next section deals with the uncertainties on total plant costs and other input parameters and how these affect production cost which is the model's output.

System sensitivity to the delivered feedstock cost is often investigated in BTL system studies. The biomass cost is the fourth most sensitive parameter, however this cost can vary enormously and certainly well outside the 10% limit tested here. As rising biomass prices can be expected in the short and medium term (see section 6.5.3.1), the conclusion of a long term biomass supply contract with fixed quantities and prices should be sought with a respectable agricultural or forest management company. If it is decided that several

companies should supply biomass during a large scale BTL plant project, a joint delivery commitment should be agreed. The next section examines uncertainties associated with feed cost in more detail.

Finally, the model is less sensitive to the interest rate, O&M costs and plant life chosen. Regarding the calculated value of O&M costs, there is some uncertainty since the estimate was based on published data (see section 6.4.2). Increased accuracy can only be achieved through very detailed analysis of the individual cost elements of O&M costs. However, this is time consuming and there are limited reliable resources on detailed O&M costs of BTL plants. Based on the demonstrated low sensitivity of the model to this parameter, there is questionable gain in the accuracy of results for such a high level of detail.

The interest rate and plant life influence the annual repayments of borrowed capital. The life of the project is largely within the control of the project developer and can be planned for. Interest rates can also be controlled by agreeing fixed rates with the lenders throughout the project's life. Thus the uncertainty associated with these parameters can be minimised.

6.7 Uncertainty analysis

6.7.1 Introduction

As discussed in section 6.4, BTL production costs were estimated using a number of technical and economic parameters assuming that these have a fixed value. However, in reality the values of these parameters which, among others, include capital costs, biomass costs and efficiency, have a certain degree of uncertainty and are not known with absolute accuracy. This results in uncertainty in the model's output (i.e. production costs) and can be reduced through acquiring more data. However, even then, the modeller can never be entirely certain of their models' estimates particularly in the case of new plant projects and technologies, such as a BTL plant, as there is no experience of a real life plant.

As mentioned above, uncertainty in the model's output results mainly from uncertain estimates of various model parameter values. Many of these values were taken from existing BTL techno-economic studies with their own estimates and assumptions and thus

they depend on the accuracy and reliability of each published study. Additionally, some model assumptions, which were presented and justified throughout this study, were made due to the lack of published data (e.g. TIGAS capital costs and product distribution). This further increases uncertainty. Uncertainty in the model's output can also result from errors in the simulation model structure compared to a real system, and approximations made by numerical methods employed in the simulation. Process simulation models are always simplifications of real processes and, hence, 'imprecision' can result. Increasing the model complexity to more closely represent the complexity of the real system may not only significantly add to the time and cost of data collection, but may also introduce even more parameters, and thus even more potential sources of uncertainty in the model's output [186].

In this study, the uncertainty analysis employed the Monte Carlo method which is commonly used for uncertainty analysis studies [187]. Each selected parameter was assigned a range of values and a probability distribution derived from the literature and industry experts. A Monte Carlo simulation of the selected input parameters to account for uncertainties was then implemented in the programming language C++. This allowed for estimates of the probability distributions of the production costs of hydrocarbon biofuels. The methodology and results of the uncertainty analysis are discussed in detail in the next sections.

It is common in other published techno-economic studies of BTL systems to assess uncertainty by sensitivity analysis where the effect on biofuel production costs of changing key model parameters is determined. This was done and discussed in the previous section. However, sensitivity analysis provides a range of output estimates without providing guidance as to the probability of a particular case occurring [186]. Additionally, uncertainty analysis repeatedly takes a high number of random samples (e.g. in this study 1,000,000 - this is set by the user) from the probability distributions of the selected uncertain parameters in order to estimate the probability distributions of the resulting outputs [186]. A sensitivity analysis deals with determenistic changes in model input values to determine the change in model output values, as shown in section 6.6. This is the first time that an uncertainty analysis is included in a published techno-economic assessment study of BTL processes for 2nd generation liquid hydrocarbon fuels.

6.7.2 Methodology

6.7.2.1 Monte Carlo simulation

There are only two published studies, both by ECN, that assess uncertainty analysis of biomass thermochemical processes [188, 189]. None of them examines transport fuels as product. The first study, which was undertaken by Calis et al. [188], is a techno-economic study of large scale (800 MW_{th}) syngas production from biomass. The second study was done by Mozaffarian and Zwart [189] and is a techno-economic assessment of SNG production systems based on biomass gasification. For their uncertainty analysis study, both studies used @RISK which is an Excel add-in software based on the Monte Carlo (MC) simulation method [188, 189].

The Monte Carlo statistical method is the most widely used means for uncertainty analysis, with applications ranging from aerospace engineering to zoology [187, 190]. This method includes random sampling from the probability distributions of a model's input parameters and repeated runs to estimate the probability distribution of the model's output. In effect, the Monte Carlo software, such as @RISK, tries a representative set combinations of the input parameter values to simulate and assess the likelihood of all possible outcomes for the model's output. The end result is a probability distribution of the model's output which allows estimation of the probability that the output will lie in a specific range. This is very useful for this study as it provides the opportunity to estimate the likelihood that BTL production costs can meet a targeted value (e.g. price of conventional fuels).

In this thesis, the uncertainty analysis study was done in the following three steps:

- Selection of the uncertain input parameters and their value range
- Choice of the probability distribution type for the selected parameters
- Implementation of the value range and probability distribution of each parameter into the Monte Carlo simulation

6.7.2.2 Uncertain parameters

The choice and the value range of the uncertain input parameters of the cost model emerges from the sensitivity analysis (see section 6.6), the literature and experts opinion. The sensitivity analysis showed that the uncertainties associated with efficiency, plant availability, capital costs, and biomass costs have a significant influence on production

costs. Therefore, these parameters were also selected for the uncertainty analysis study. Operating costs and interest were also selected as there is also some uncertainty associated with these two parameters. O&M costs were taken as a percentage of the TPC (5% TPC – see section 6.4.2.2) which was based on reported costs of other published studies. The interest for capital repayment is likely to be higher than 10% due to the fact that a BTL plant has never been built before and thus there is higher risk for the lender. The selected uncertain parameters together with their value range are shown in Table 6-10.

Table 6-10: Selected uncertain input parameters of the cost model from literature and experts

Parameter	Base assumption/estimation	Range	Source
Biomass cost	58.69 £/dry t	± 50%	[33]
Literature installed costs	See Table 6-2	± 30%	[90, 114]
O&M cost (gasification)	5% TPC	3-7%	[189]
Maintenance cost (fast pyrolysis)	2.5% TPC	2-3%	[16, 90, 92]
Fixed costs	2% TPC	1.5-2.5%	[16, 90, 92]
Interest	10%	8-15%	[33]
Land	6% TPEC	4-8%	[95]
Power plant installed cost	14% other installed costs	11-16%	[90, 92, 114]
Scale factor	0.65	0.6-0.7	[99]
Plant availability	8000 hrs/year	7008-8322	[92, 96]
Efficiency (GJ/h)	See section 5.12	± 20%	[33]

According to Larson et al. [114] and Swanson et al. [90] accuracy of capital costs results is usually ± 30%. Therefore, for the installed costs, which were based on other literature costs (see section 6.3), a ± 30% deviation from their default value was assumed.

As discussed in section 6.4.3 and 6.6, biomass prices can vary significantly with no systematic pattern. Thus, a large deviation of ± 50% was selected to express the high uncertainty associated with this parameter.

The process efficiency (GJ/h) was assigned a ± 20% deviation from the default value which was estimated in IPSEpro. The efficiency results presented in section 5.12 showed that they are consistent with other published studies of BTL systems, thus a larger deviation than ± 20% was not needed.

The uncertainty analysis study was done for the Excel cost models only, thus it did not include any parameters of the IPSEpro models of the selected BTL systems. However, since the capital costs are based on IPSEpro process simulation parameters (e.g. scale, oxygen requirements) the cost uncertainties in Table 6-10 may be considered to reflect the IPSEpro model uncertainties to some degree. Future studies will explicitly address the uncertainty of process simulation parameters in addition to cost parameters.

6.7.2.3 Probability distributions

For all the selected uncertain parameters in Table 6-10, bounded normal probability distributions (i.e. normal distributions constrained to lie in the ranges specified in Table 6-10) were chosen. In uncertainty analyses, the normal distribution is used for the probability distribution of the input parameters when the most likely values for the input parameters can be estimated but fluctuations around these values are expected [191]. As discussed in section 5.12.4 and 6.5, the performance and cost results of this study were consistent with those of other techno-economic studies of BTL systems. For this reason it is more likely that the values of the model input parameters will be closer to their default value. In addition, both ECN studies [188, 189] discussed in the section 6.7.2.1 used the normal distribution for their uncertain parameters. Mozaffarian and Zwart [189] mainly used the PERT distribution which is similar to a bounded normal distribution as it is also requires a minimum, a maximum and a most likely value [192]. However, no reason was provided for choosing the PERT distribution over the bounded normal distribution. Therefore, in this study, the probability distribution selected for the uncertain parameters of the cost model was the bounded normal distribution. All of the normal distributions in this study were parameterized such that the distance between the most likely value and the upper end of the range was equal to three standard deviations.

To estimate the probability distributions of the production costs, the normal probability distributions of the uncertain parameters were simulated as part of a Monte Carlo simulation. Because uncertainly analysis software, such as @RISK and RiskAmp, was not available at Aston University, the simulation was implemented in C++. This was done in collaboration with the Computer Science Department of Aston University.

6.7.3 Results

The cumulative probability distributions of biofuel production costs of the CFB concepts and the EF concepts are shown in Figure 6-6 and Figure 6-7, respectively. For the CFB-FT concept, which was the most economic system (see section 6.5.3), the 90% confidence interval of production cost is 12.5–18 £/GJ, compared to the deterministic estimate of 14.65 £/GJ. In other words, the actual value has 90% chance to be within the range of 12.5 to 18 £/GJ. Similarly, it is observed that the chance that the cost exceeds 17 £/GJ in this case, is approximately 10%. This shows how important the economic assumptions are in estimating the economic feasibility of a BTL plant.

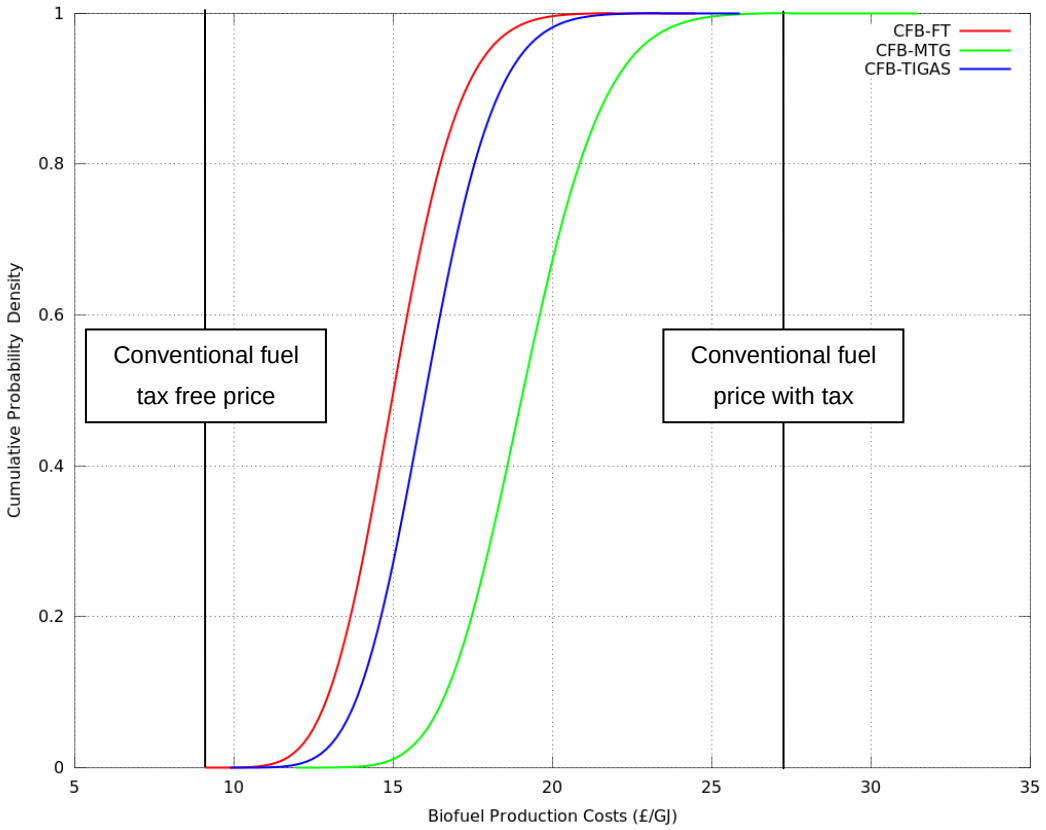

Figure 6-6: Cumulative probability of biofuel production costs (£/GJ) of the CFB concepts

As discussed in section 6.5.3.2, the 2009 refinery gate (tax-free) price of fossil transport fuels was 8.7 £/GJ on average. The chance that the biofuel production cost of the CFB-FT concept will meet this price is very low (close to zero). However, from Figure 6-6, it can be

seen that there is a 50% chance that the production cost of the CFB-FT concept, will be less than 14.65 £/GJ. Therefore, if biofuel production costs were reduced from this level to 8.7 £/GJ (approximately 40% reduction) through capital, biomass, manufacturing and/or tax credits, there is a 50% chance that they will meet or exceed the conventional fuel prices. Additionally, the conventional transport fuel tax rate in the UK in 2009 was approximately 67.7% on average [178]. Therefore, the conventional fuel price, including tax was approximately 27 £/GJ (see Figure 6-6). If biofuels from the CFB-FT concept were to have 50% chance to meet this price then a tax take of 45.7% would be required. This is 22% less than the conventional fuel tax take (67.7%). Therefore, if the government tax take (i.e. the amount of tax that that the government receives per GJ of fuel produced) was reduced by approximately 32.5%, biofuels through the CFB-FT route could be competitive with conventional transport fuels. This is promising based on the current political climate for biofuel subsidies which was discussed in section 6.5.3.2.

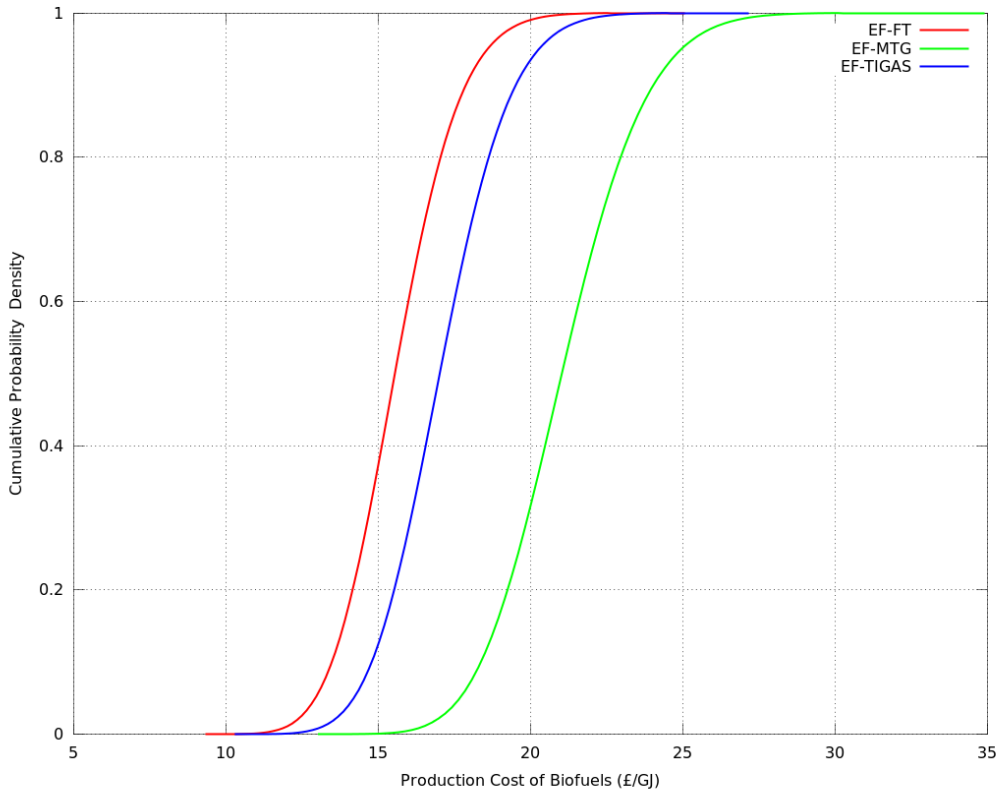

Figure 6-7: Cumulative probability of biofuel production costs (£/GJ) of the EF concepts

For the CFB-TIG, which was the most economic concept for gasoline production, the 90% confidence interval of production cost is 13.5–19 £/GJ, compared to the deterministic estimate of 15.64 £/GJ. The probability that the gasoline production costs of this concept meet the 2009 refinery gate price of gasoline (8.6 £/GJ) is zero. If production costs of this concept were reduced from the initial estimate of 15.64 £/GJ to 8.7 £/GJ (approximately 44% reduction), there is a 50% chance that they will meet or exceed the conventional gasoline price. Similarly to the CFB-FT concept, a tax rate of 42% would be required if gasoline from the CFB-TIG was to have a 50% chance to meet the conventional gasoline tax price. Thus a government tax take reduction of approximately 38% would be required for the CFB-TIG gasoline to compete economically with conventional gasoline.

For the most economic EF concept, which was the EF-FT concept (see section 6.5.3), the 90% confidence interval of production cost is 12.9–18.6 £/GJ, compared to the deterministic estimate of 15.18 £/GJ. Additionally, the actual value has 44% chance to be within the range of 14 to 16 £/GJ, which shows the impact of uncertainties of the model's input parameters on the estimated production cost. If production costs of the EF-FT concept were reduced from the initial estimate of 15.18 £/GJ to 8.7 £/GJ (approximately 43% reduction), there is a 50% chance that they will meet or exceed the conventional transport fuel price. A tax rate of 43.8% would be required if biofuels from the EF-FT were to have a 50% chance to meet the conventional fuel tax price. Therefore, if the government tax take was reduced by approximately 35%, biofuels through the EF-FT route could be competitive with conventional transport fuels.

Figure 6-8 shows the cumulative probability of biofuel production costs of the bio-oil gasification concepts. For the FP-FT concept, which was the most economic bio-oil gasification system, the actual value has 90% chance to be within 24-34 £/GJ.

The range is wider than the equivalent biomass gasification concept (EF-FT). However, since the range will increase with the mean (initial estimated value) it is more appropriate to compare the relative range of the uncertainties (i.e. the range as a proportion of the mean). For the FP-FT concept there is a 36% relative uncertainty which is similar to the EF-FT concept's value of 38%.

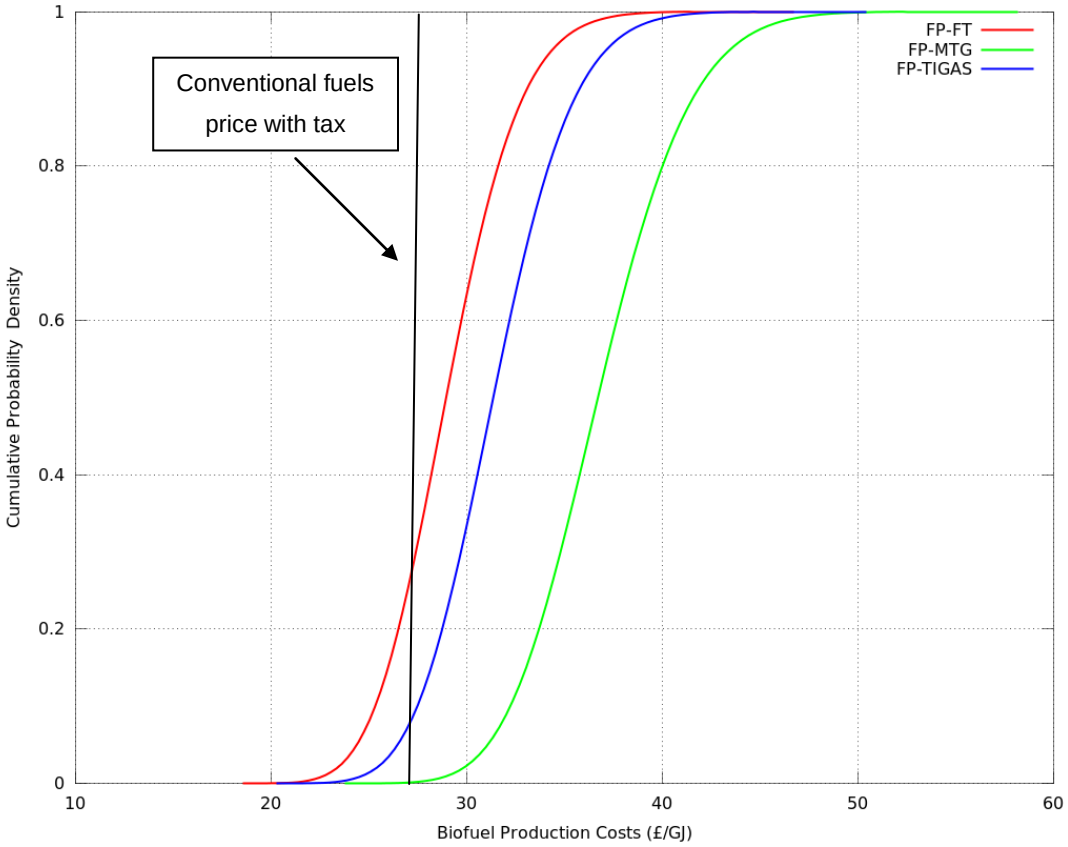

Figure 6-8: Cumulative probability of biofuel production costs (£/GJ) of the bio-oil gasification concepts

The production costs of the FP-FT concept need to be reduced by 70% in order to have a 50% chance to meet the conventional fuel prices. This is a very high reduction and it is questionable if it can be achieved through subsidies only. There is a 27 % chance that the production cost of this concept will meet or exceed the conventional fuel price including tax (27 £/GJ). There is zero chance that it will meet the conventional tax free fuel prices (8.7 £/GJ). Therefore, it is very unlikely that this and the other bio-oil gasification concepts can compete with conventional transport fuels at the current time.

Table 6-11 shows, for each solid biomass gasification concept, the tax take reduction required for biofuels to meet the conventional fuel prices including tax. It can be seen that

the most expensive option (EF-MTG) would need approximately twice as much tax take reduction as the CFB-FT concept which was the most economic BTL plant concept.

Table 6-11: Tax take reduction (as a percentage of the 2009 tax take for conventional fuels) necessary for biofuels to compete with conventional fuels

Concept	Tax take reduction (%) from 2009 tax take
CFB-FT	32.5
CFB-MTG	53.8
CFB-TIG	38
EF-FT	35
EF-MTG	64.4
EF-TIG	43.2

7 CONCLUSIONS

The aim of this work was to calculate, evaluate and compare the costs and performance of thermochemical routes from solid biomass to 2nd generation liquid transport fuels, known as Biomass-To-Liquids (BTL) processes. The project was undertaken to provide a consistent and thorough review of the full range of these pathways to compare alternative technologies within them in order to identify the most promising opportunities that deserve closer attention. The scope was limited to hydrocarbon products (diesel, gasoline and kerosene) as these can be readily incorporated and integrated into conventional markets and supply chains while alcohols and ethers have more limited short term prospects in the UK and European transport fuel infrastructures.

Nine BTL plant concepts were selected which were based on entrained flow and circulating fluidised bed gasification of wood biomass or bio-oil. Fuel synthesis technologies included Fischer-Tropsch synthesis, methanol synthesis followed by the Methanol-to-Gasoline (MTG) process and the Topsoe integrated gasoline (TIGAS) synthesis. This was the first time that these three fuel synthesis technologies were compared in terms of performance and costs in a published techno-economic assessment study of biofuel systems.

All BTL concepts were modelled using the equation oriented process simulation software IPSEpro in order to determine mass balances, energy balances, and product distributions. The process simulation results showed the following:

- Fischer-Tropsch synthesis looks the most promising fuel synthesis technology for commercial production of liquid hydrocarbon fuels since it achieved higher efficiencies than the TIGAS and MTG. This is due to the additional synthesis steps required in TIGAS and especially in the MTG process as each synthesis step results in lower mass yields and thus lower energy conversion efficiencies.
- The CFB-FT concept showed the highest energy efficiency and mass yield at approximately 47.6% and 20.6%, respectively.
- The EF-MTG concept was the least promising solid biomass gasification concept in terms of energy and mass yields (38% and 17.8%, respectively).

- CFB gasification resulted in slightly higher energy efficiencies by 2.6–5.5% than entrained flow gasification. This was due to the loss of energy during quenching and cooling of the syngas after the entrained flow gasifier.
- Bio-oil gasification concepts showed significantly lower energy efficiencies (14-17%) than the solid biomass gasification concepts due to the additional thermal conversion step of fast pyrolysis. It is therefore questionable whether bio-oil gasification could ever be competitive, in terms of efficiency, with solid biomass gasification.
- This study's results on the performance of BTL plant concepts are consistent with those from other modelling studies of BTL systems.

An economic assessment of the BTL concepts modelled was also carried out in order to identify the most promising BTL processes in terms of production costs. Another important aim was to examine whether BTL plants could compete economically with conventional transport fuels plants. 2009 was the base year for the economic analysis which included estimates of capital, operating and production costs for each of the nine BTL concepts. A sensitivity analysis was also carried out to investigate the impact of different cost parameters on the production costs of BTL plants. Similar techno-economic studies of BTL plants which are publicly available have not dealt with uncertainty in their cost models' input parameters. Rather than assuming that the input parameters are known with an absolute accuracy, one should have the model account for uncertainties in the input parameters. To this end, an uncertainty analysis based on the Monte Carlo statistical method was carried out to examine how the uncertainty in the input parameters of the cost model could affect the output (i.e. production cost) of the model. The results of the economic assessment study showed the following:

- The Fischer-Tropsch synthesis was the most economic option of all three fuel synthesis technologies as it gave the lowest capital, operating and production costs.
- The major process areas of capital investment for all BTL concepts based on solid biomass gasification, were the gasification and gas clean-up area and the fuel synthesis area.
- CFB gasification was more capital intensive due to the need for a tar cracker and the additional heat exchange equipment required for syngas cooling.

- The MTG process was the most expensive fuel synthesis option due to its increased complexity and low efficiencies.
- Bio-oil gasification for biofuel production gave slightly higher capital and operating costs than the equivalent solid biomass concepts. However, the conversion efficiency was much lower thus leading to much higher production costs. Therefore, it seems questionable if fast pyrolysis coupled with gasification will ever be an economically viable option for the production of liquid hydrocarbon fuels.
- The CFB-FT concept was the most promising BTL concept as it gave the lowest production costs (14.65 £/GJ), whereas the least economically attractive concept based on solid biomass gasification was the EF-MTG concept (20.48 £/GJ).
- A biomass subsidy of approximately £55/t of dried wood would be required to meet the conventional fuel prices. However, it is unlikely that this high subsidy will be given to large scale BTL plants.
- Clear political parameters which need to be stable over a period of time of at least 20 years are necessary if investors and lenders are to provide long term financing for the first large scale BTL plant.
- Process efficiency has the most sensitive effect on biofuel production costs, thus improving process performance should be an early priority.
- Plant availability is the second most sensitive item in production costs thus it is imperative to the viability of commercial BTL plants that the plant operating hours are as high as possible to maximise annual production in order to reduce production costs.
- Based on the initial estimates of production costs there is a very low probability that biofuel production costs will meet the price of conventional fuels. If biofuel production costs were reduced by 40% through capital, biomass, manufacturing and tax subsidies, there is a 50% chance that they will meet or exceed the conventional fuel prices.
- Transport biofuels could be competitive with conventional fuels if government tax was reduced by approximately 32.5%.

This study was based on the fuel market in the UK so some of its findings may not be relevant to other countries. The study assumed that the gasification plant was located in the centre of the area that provided it with biomass (or bio-oil), thus the findings may be different for plants that use imported biomass or biomass from across the country.

Extensive use is made of published data which was taken from existing BTL techno-economic studies with their own estimates and assumptions. This affects the overall results which highly depend on the accuracy and reliability of each published study. Additionally, there was limited published information on the MTG and especially the TIGAS process thus some assumptions had to be made. This further increases the uncertainty of the performance and economic results of these fuel synthesis technologies.

While the evaluation showed that none of the BTL systems are directly competitive on price with conventional large scale fossil fuel plants (which enjoy the benefits of low feedstock costs and strong economies of scale), large scale biofuel production can be made competitive through a combination of subsidies and tax reduction. Subsidy schemes are now in place in many countries in Europe and the UK but they rely on public and political support for their long term implementation. In addition, future fossil fuel prices rises and environmental taxes would enhance the competitiveness of biofuels.

8 RECOMMENDATIONS FOR FUTURE WORK

The recommendations resulting from the work reported in this thesis are as follows:

- Evaluation of other biomass feedstocks. This may require additions and changes to the current biomass preparation and pre-treatment models on IPSEpro.
- Investigation of different scales and their effects on the performance and costs of BTL plants.
- Because of time and resource constraints, the techno-economic study did not include electricity production and heat integration, thus a complete heat exchange network for heat recovery was not conceptualized. This could be addressed in the future and relevant models could be built on IPSEpro.
- Due to lack of published data some processes such as TIGAS could not be modelled rigorously and can be improved with detailed mass and energy flows and costs when more information is available. More detailed modelling will likely result in changes to economic components such as capital and operating costs.
- Heat for the fast pyrolysis process was supplied by combustion of the char and off-gas. It is likely that the fast pyrolysis process could be more cost-effective if the char was sold as a by-product and another energy source was used in the process. Future work could consider the various options available.
- Evaluation of atmospheric gasification and comparison with pressurised gasification systems.
- Modelling and economic analysis of other fuel synthesis technologies, such as MOGD, MtSynfuels and bio-oil upgrading routes, to highlight their benefits and drawbacks in comparison with the BTL systems already evaluated in this study.
- Inclusion of torrefaction for biomass pre-treatment as it gives a dry and grindable product which makes it suitable for entrained flow gasification. Heat integration of the process could be examined to see whether or not the off-gas alone can cover the heat requirements of the process as claimed by ECN.
- The gasification of bio-oil/char slurry could also be examined and compared with bio-oil and solid biomass gasification.

- The uncertainty analysis study did not include any parameters of the IPSEpro models of the selected BTL systems. Future studies could explicitly address the uncertainty of process simulation parameters in addition to cost parameters.
- Different operations in the process chain have different degrees of risk and uncertainty. For example, the development and demonstration of pressurized, oxygen-blown CFB gasification of biomass involves significantly greater technical risks than EF gasification which is already employed in large scale coal plants. Therefore, it would be possible to expand the uncertainty analysis to include risks and uncertainties associated with different technologies within a BTL process. These uncertainties could be quantified and their impact on production costs could be investigated.

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Appendix A. IPSEpro examples and list of models

Available units:

PG_comb_dfb	combustion chamber in dual fluidized bed gasification process
PG_comb_g	gas combustion chamber
PG_comb_o	organic fuel combustion chamber
PG_compr_g	gas compressor
PG_compr_w	steam compressor
PG_cond_gw	selective condenser / gas dryer
PG_conv_oo	organic - organic converter
PG_drum_w	steam drum
PG_dryer	fuel dryer
PG_gasengine	gas engine
PG_gasif_dfb	gasifier in dual fluidized bed gasification process
PG_gasif_o	gasifier
PG_heat_sink_g	heat sink for gas
PG_heat_sink_w	heat sink for water
PG_heat_source_g	heat source for gas
PG_heat_source_w	heat source for water
PG_htex_gg	gas - gas heat exchanger
PG_htex_go	gas - organic heat exchanger
PG_htex_gw	gas - water/steam heat exchanger
PG_htex_oo	organic - organic heat exchanger
PG_htex_sw	solid - water/steam heat exchanger
PG_htex_wo	water/steam - organic heat exchanger
PG_htex_ww	water/steam - water/steam heat exchanger
PG_inj_sg	solids into gas injector
PG_inj_so	solids into organic injector
PG_inj_wg	water/steam into gas injector
PG_inj_wo	water into organic injector
PG_loop_g	gas loop connector
PG_loop_o	organic loop connector
PG_loop_w	water/steam loop connector
PG_mixer_g	gas stream mixer
PG_mixer_o	organic stream mixer
PG_mixer_s	solid stream mixer
PG_mixer_w	water/steam stream mixer
PG_monitor_ambient	ambient air monitor
PG_monitor_g	gas stream monitor
PG_monitor_o	organic stream monitor
PG_monitor_s	solid stream monitor
PG_monitor_w	water/steam stream monitor
PG_orc_bbox	organic rankine cycle black box
PG_oxid_react	gas oxidation reactor
PG_pipe_g	gas pipe
PG_pipe_w	water/steam pipe

PG_pump_o	organic pump
PG_pump_w	water pump
PG_quench_w	water quench
PG_scrubber_go	organic solvent gas scrubber
PG_sep_gs	gas - solid separator
PG_sep_os	organic - solids separator
PG_sep_ow	organic - water separator
PG_sink_ambient	gas sink to ambient environment
PG_sink_g	gas sink
PG_sink_o	organic sink
PG_sink_s	solids sink
PG_sink_w	water/steam sink
PG_source_ambient	ambient air gas source
PG_source_g	gas source
PG_source_o	organic source
PG_source_s	solids source
PG_source_w	water/steam source
PG_splitter_g	gas stream splitter
PG_splitter_o	organic stream splitter
PG_splitter_s	solids stream splitter
PG_splitter_w	water/steam stream splitter
PG_steam_ref	steam reforming reactor
PG_turbine_g	gas turbine
PG_turbine_w	steam turbine
generator	generator
motor	motor

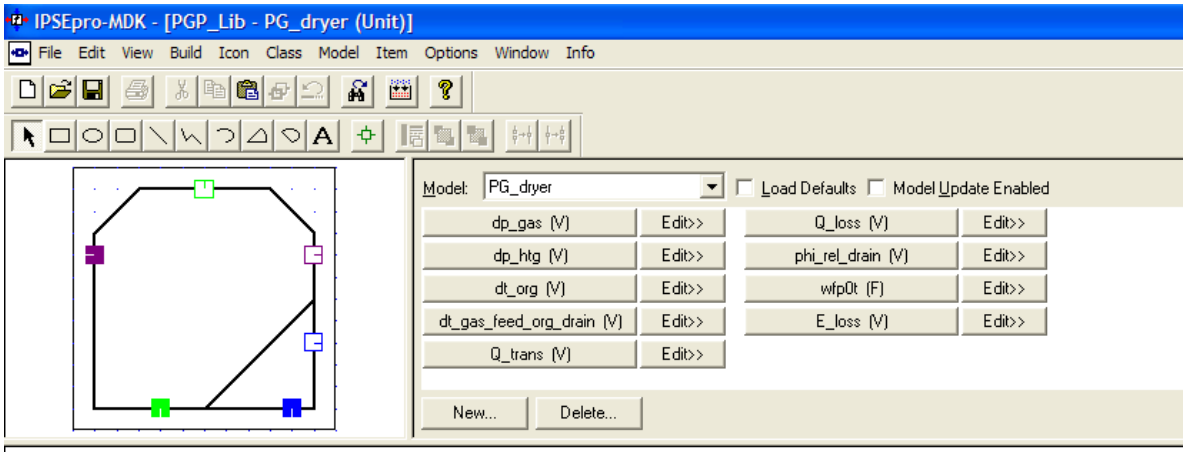
Available stream connections:

PG_stream_g	gas stream
PG_stream_o	organic stream (solid or liquid fuels, solvent, or heat carrier oil)
PG_stream_s	(inorganic) solids stream
PG_stream_w	water/steam stream

Available compositions:

PG_ambient	ambient conditions
PG_comp_g	gas composition
PG_comp_o	organic composition
PG_comp_s	solids composition

Example of an IPSEpro model (dryer) on the MDK




```
# ************************************************************************************************************************************************************
# ************************************************************  EQUATION  SECTION  ************************************************************
# ************************************************************************************************************************************************************
# Unit PG_dryer describes a fuel stream dryer with either direct or indirect heating
# The composition of the fuel stream at drain is the same as in feed, there are no hydrocarbons, CO, dust or something else produced and emitted with dryer exhaust air
# The heating water/steam stream is optional
# The dryer air feed is optional
# Thereby it is possible to model convective drying, indirectly heated contact drying, and combinations of the mentioned methods

# Energy Balance

# Case 1: gas feed connected
ifl ref(feed_gas) then
                    f1htotal:   drain_gas.massflow*drain_gas.h_total + drain_org.massflow*drain_org.h_total =
                                feed_gas.massflow*feed_gas.h_total + feed_org.massflow*feed_org.h_total + (Q_trans - Q_loss)*3600.0;

# Case 2: no gas feed connected
elsel
                    f2htotal:   drain_gas.massflow*drain_gas.h_total + drain_org.massflow*drain_org.h_total =
                                feed_org.massflow*feed_org.h_total + (Q_trans - Q_loss)*3600.0;
endifl


# Mass balance equations

# Equations for optional heating water/steam stream

ifl ref(feed_htg) && ref(drain_htg) then

  fmassheating:   feed_htg.massflow = drain_htg.massflow;
```

Appendix B. Average enthalpy calculation for FT model substances

$$H_i(T) = H(T,n) \;=\; \Delta h^0_{f,298} \;+ \int_{298.15}^{T} C_p(T,n)\cdot dT =$$

$$k_1 + k_2\cdot n + \left[(n-2)\cdot\left(0.0354\cdot\frac{T^2}{2} + 20.21\cdot T\right) + \;2\cdot\left(0.1205\cdot\frac{T^2}{2} - 1.4721\cdot T\right)\right]_{298.15}^{T} \quad (1)$$

Rearranging $C_p(T,n)$ we get:

$$C_p(T,n) = \;2\cdot T\;\cdot\;(1.77\;\cdot\;n\;+\;8.51)\cdot\;10^{-2} + \;20.2\;\cdot\;n - \;43.4 \quad (2)$$

Calculating the indefinite integral:

$$y(T,n) = \int C_p(T,n)dT \;=\; T^2\cdot(1.77\cdot n + 8.51)\cdot 10^{-2} + T\cdot(20.2\cdot n - 43.4) \quad (3)$$

giving us the enthalpy equation:

$$H(T,n) = \frac{(k_1 \;+\; k_2\cdot n)\cdot\;10^3 + \;y(T,n) - y(298.15,n)}{14\cdot n + 2} \quad (4)$$

where $14\cdot n + 2$ is the molecular weight (g/mol) of the n-alkanes (C_nH_{2n+2}).

Now, let:

$$\widehat{H}(T) = \;k_2\cdot 10^3 + \;(T^2 - 298.15^2)\cdot 1.77\cdot 10^{-2} + (T - 298.15)\cdot 20.2 \quad (5)$$
$$E_T(T) = \;k_1\cdot 10^3 + \;(T^2 - 298.15^2)\cdot 8.51\cdot 10^{-2} - (T - 298.15)\cdot 43.4 \quad (6)$$
$$E_n(n) = 14\cdot n + 2 \quad (7)$$

Equation (4) is arranged to give:

$$H(T,n) = \frac{n\cdot\widehat{H}\;(T) + E_T(T)}{E_n(n)} \quad (8)$$

Now, let $p(n)$ be the mass fraction (wt%) of the hydrocarbon with chain length n. Let n_{min} and n_{max} be the minimum (five) and maximum chain-length (thirty five), respectively. The average enthalpy at temperature T is given by:

$$\overline{H}(T) = \sum_{n=n_{min}}^{n_{max}} p(n)H(T,n)$$

$$= \sum_{n=n_{min}}^{n_{max}} p(n) \cdot \frac{n \cdot \widehat{H}(T) + E_T(T)}{E_n(n)}$$

$$= \widehat{H}(T) \cdot \sum_{n=n_{min}}^{n_{max}} \frac{n \cdot p(n)}{E_n(n)} + E_T(T) \cdot \sum_{n=n_{min}}^{n_{max}} \frac{p(n)}{E_n(n)} \quad (9)$$

Appendix C. Cost results

APPENDIX C.1: Capital, operating and production costs of the evaluated BTL concepts

EF-FT concept

Table C-1: Costs results for the EF-FT concept

CAPITAL COST		
	Cost (£)	%
Biomass preparation & RSH	13,602,783	5.0
Gasification & gas cleaning	40,445,361	14.9
Gas conditioning	20,139,359	7.4
FT synthesis & upgrading	47,966,668	17.6
Air separation	21,357,929	7.9
Power plant	20,091,694	7.4
Other direct costs	29,461,220	10.8
Indirect costs	78,981,142	29.0
Total	**272,046,155**	100.0

OPERATING COST		
	Cost (£)	%
O&M	10,881,846	18.6
Power	2,720,462	4.7
Fixed	5,440,923	9.3
Biomass	39,439,680	67.4
Total	**58,482,911**	100.0

PRODUCTION COST		
	£/GJ	%
Capital	5.36	35.3
O&M	3.20	21.1
Biomass	6.62	43.6
Total	**15.18**	100.0

EF-MTG concept

Table C-2: Costs results for the EF-MTG concept

CAPITAL COST		
	Cost (£)	%
Biomass preparation & RSH	13,602,783	4.0
Gasification & gas cleaning	40,445,361	12.0
Gas conditioning	20,139,359	6.0
Methanol synthesis	39,947,545	11.8
MTG & upgrading	42,343,659	12.6
Air separation	21,357,929	6.3
Power plant	24,897,129	7.4
Other direct costs	36,507,613	10.8
Indirect costs	97,871,473	29.0
Total	**337,112,852**	100

OPERATING COST		
	Cost (£)	%
O&M	13,484,514	21.4
Power	3,371,129	5.3
Fixed	6,742,257	10.7
Biomass	39,439,680	62.6
Total	**63,037,580**	100

PRODUCTION COST		
	£/GJ	%
Capital	7.90	38.6
O&M	4.71	23.0
Biomass	7.87	38.4
Total	**20.48**	100

EF-TIG concept

Table C-3: Costs results for the EF-TIG concept

CAPITAL COST		
	Cost (£)	%
Biomass preparation & RSH	13,602,783	5.1
Gasification & gas cleaning	40,445,361	15.3
Gas conditioning	20,139,359	7.6
TIGAS & upgrading	44,218,909	16.7
Air separation	21,357,929	8.1
Power plant	19,567,008	7.4
Other direct costs	28,691,852	10.8
Indirect costs	76,918,582	29.0
Total	**264,941,784**	100.0

OPERATING COST		
	Cost (£)	%
O&M	10,597,671	18.3
Power	2,649,418	4.6
Fixed	5,298,836	9.1
Biomass	39,439,680	68.0
Total	**57,985,605**	100.0

PRODUCTION COST		
	£/GJ	%
Capital	5.80	34.9
O&M	3.46	20.8
Biomass	7.36	44.3
Total	**16.62**	100.0

CFB-FT concept

Table C-4: Costs results for the CFB-FT concept

CAPITAL COST		
	Cost (£)	%
Biomass preparation & RSH	12,341,894	4.4
Gasification & gas cleaning	55,280,179	19.6
Gas conditioning	18,036,856	6.4
FT synthesis & upgrading	45,745,324	16.2
Air separation	17,350,199	6.2
Power plant	20,825,623	7.4
Other direct costs	30,537,408	10.8
Indirect costs	81,866,244	29.0
Total	**281,983,728**	100.0

OPERATING COST		
	Cost (£)	%
O&M	14,099,186	23.8
Fixed	5,639,675	9.5
Biomass	39,439,680	66.6
Total	**59,178,541**	100.0

PRODUCTION COST		
	£/GJ	%
Capital	5.26	35.9
O&M	3.13	21.4
Biomass	6.26	42.7
Total	**14.65**	100.0

CFB-MTG concept

Table C-5: Costs results for the CFB-MTG concept

CAPITAL COST		
	Cost (£)	%
Biomass preparation & RSH	12,341,894	3.4
Gasification & gas cleaning	55,280,179	15.4
Gas conditioning	18,036,856	5.0
Methanol synthesis	39,947,545	11.1
MTG & upgrading	46,279,333	12.9
Air separation	17,350,199	4.8
Power plant	26,493,041	7.4
Other direct costs	38,847,760	10.8
Indirect costs	104,145,058	29.0
Total	**358,721,866**	100.00

OPERATING COST		
	Cost (£)	%
O&M	14,348,875	22.2
Power	3,587,219	5.6
Fixed	7,174,437	11.1
Biomass	39,439,680	61.1
Total	**64,550,211**	100.0

PRODUCTION COST		
	£/GJ	%
Capital	7.33	39.5
O&M	4.37	23.5
Biomass	6.86	37.0
Total	**18.56**	100.0

CFB-TIG concept

Table C-6: Costs results for the CFB-TIG concept

CAPITAL COST		
	Cost (£)	%
Biomass preparation & RSH	12,341,894	4.3
Gasification & gas cleaning	55,280,179	19.4
Gas conditioning	18,036,856	6.3
TIGAS & upgrading	47,267,532	16.6
Air separation	17,350,199	6.1
Power plant	21,038,732	7.4
Other direct costs	30,849,898	10.8
Indirect costs	82,703,983	29.0
Total	**284,869,274**	100.0

OPERATING COST		
	Cost (£)	%
O&M	11,394,771	19.2
Power	2,848,693	4.8
Fixed	5,697,385	9.6
Biomass	39,439,680	66.4
Total	**59,380,529**	100.0

PRODUCTION COST		
	£/GJ	%
Capital	5.64	36.0
O&M	3.36	21.5
Biomass	6.64	42.5
Total	**15.64**	100.0

FP-FT concept

Table C-7: Costs results for the FP-FT concept

CAPITAL COST		
	Cost (£)	%
Biomass preparation & RSH	12,575,241	3.7
Fast pyrolysis	78,891,010	23.0
Gasification & gas cleaning	30,786,540	9.0
Gas conditioning	15,329,846	4.5
FT synthesis & upgrading	36,511,671	10.6
Air separation	18,008,299	5.3
Power plant	14,089,090	4.1
Other direct costs	37,130,306	10.8
Indirect costs	99,540,819	29.0
Total	**342,862,821**	100.0

OPERATING COST		
	Cost (£)	%
O&M	15,214,299	23.5
Power	2,506,015	3.9
Fixed	6,439,045	10.0
Bi-oil transport	3,625,000	5.6
Biomass	36,899,520	57.0
Total	**64,683,880**	100.0

PRODUCTION COST		
	£/GJ	%
Capital	10.79	38.4
O&M	7.45	26.5
Biomass	9.89	35.2
Total	**28.13**	100.0

FP-MTG concept

Table C-8: Costs results for the FP-MTG concept

CAPITAL COST		
	Cost (£)	%
Biomass preparation & RSH	12,575,241	3.2
Fast Pyrolysis	78,891,010	20.2
Gasification & gas cleaning	30,786,540	7.9
Gas conditioning	15,329,846	3.9
Methanol synthesis	30,407,608	7.8
MTG & upgrading	31,652,353	8.1
Air separation	18,008,299	4.6
Power plant	17,665,850	4.5
Other direct costs	42,375,046	10.8
Indirect costs	113,601,188	29.0
Total	**391,292,982**	100.0

OPERATING COST		
	Cost (£)	%
O&M	17,151,506	25.2
Power	2,990,317	4.4
Fixed	7,407,649	10.9
Bi-oil transport	3,625,000	5.3
Biomass	36,899,520	54.2
Total	**68,073,991**	100.0

PRODUCTION COST		
	£/GJ	%
Capital	14.35	40.3
O&M	9.73	27.3
Biomass	11.52	32.4
Total	**35.60**	100.0

FP-TIG concept

Table C-9: Costs results for the FP-TIG concept

CAPITAL COST		
	Cost (£)	%
Biomass preparation & RSH	12,575,241	3.7
Fast Pyrolysis	78,891,010	23.5
Gasification & gas cleaning	30,786,540	9.2
Gas conditioning	15,329,846	4.6
TIGAS & upgrading	32,902,065	9.8
Air separation	18,008,299	5.4
Power plant	13,583,745	4.0
Other direct costs	36,389,299	10.8
Indirect costs	97,554,291	29.0
Total	**336,020,337**	100.0

OPERATING COST		
	Cost (£)	%
O&M	14,940,600	23.3
Power	2,437,590	3.8
Fixed	6,302,196	9.8
Bi-oil transport	3,625,000	5.6
Biomass	36,899,520	57.5
Total	**64,204,906**	100.0

PRODUCTION COST		
	£/GJ	%
Capital	11.60	38.1
O&M	8.03	26.3
Biomass	10.84	35.6
Total	**30.47**	100.0

APPENDIX C.2: Sensitivity analysis results

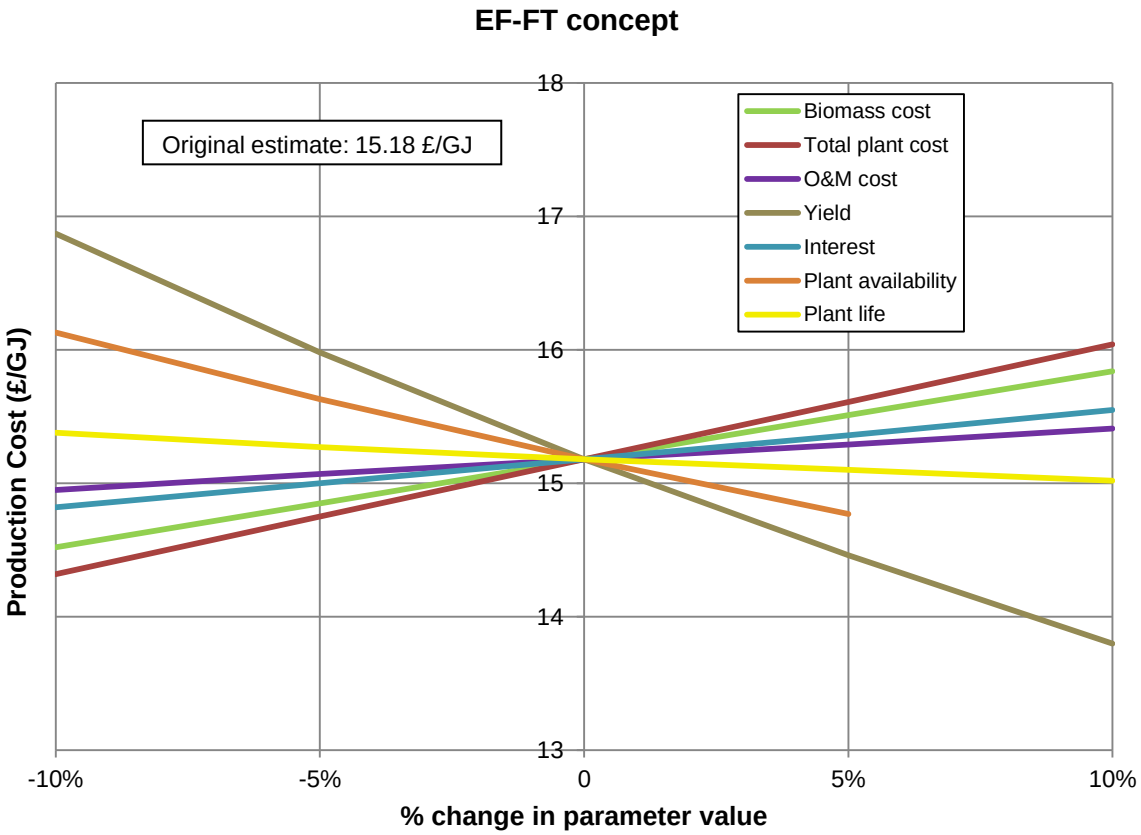


Figure C-1: Sensitivity of biofuels production cost of the EF-FT concept

Table C-10: Production costs of the EF-FT concept as a result of parameters' variations

	-10%	-5%	0	5%	10%
Biomass cost	14.52	14.85	15.18	15.51	15.84
Total plant cost	14.32	14.75	15.18	15.61	16.04
O&M cost	14.95	15.07	15.18	15.29	15.41
Yield	16.87	15.98	15.18	14.46	13.80
Interest	14.82	15.00	15.18	15.36	15.55
Plant availability	16.13	15.63	15.18	14.77	-
Plant life	15.38	15.27	15.18	15.1	15.02

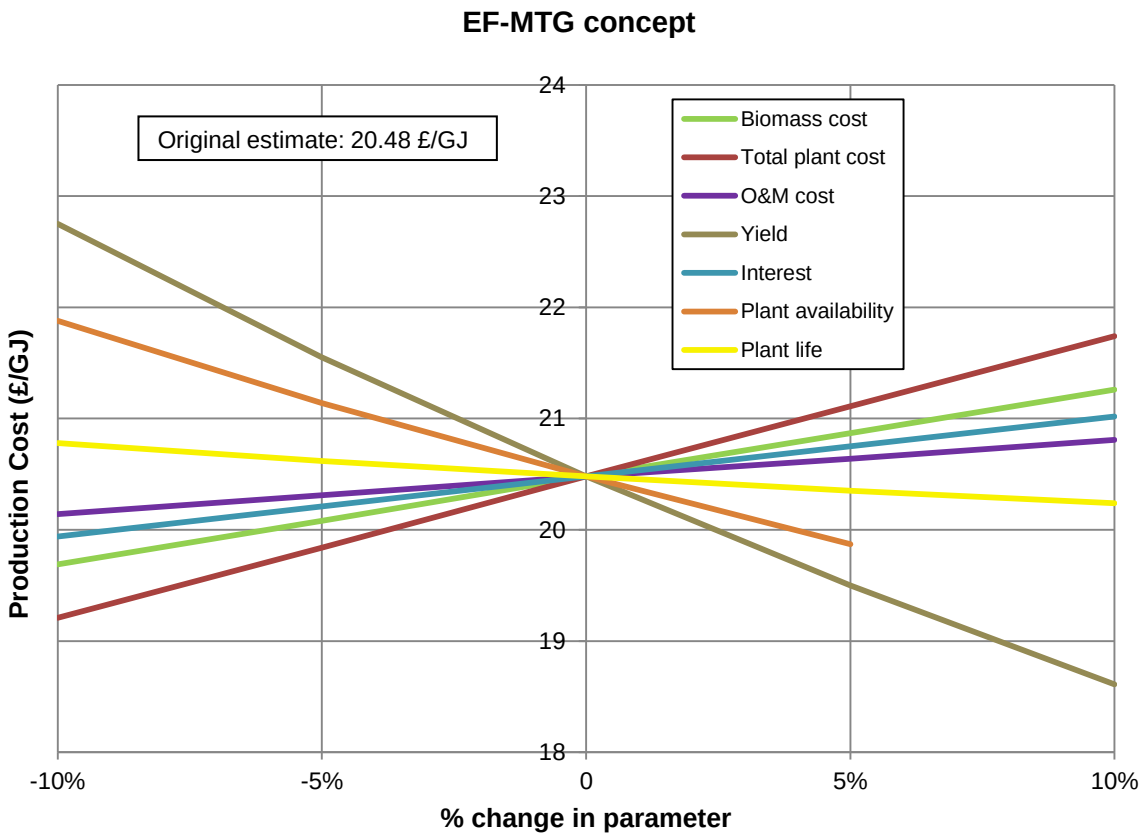


Figure C-2: Sensitivity of biofuels production cost of the EF-MTG concept

Table C-11: Production costs of the EF-MTG concept as a result of parameters' variations

	-10%	-5%	0	5%	10%
Biomass cost	19.69	20.08	20.48	20.87	21.26
Total plant cost	19.21	19.84	20.48	21.11	21.74
O&M cost	20.14	20.31	20.48	20.64	20.81
Yield	22.75	21.55	20.48	19.5	18.61
Interest	19.94	20.21	20.48	20.75	21.02
Plant availability	21.88	21.14	20.48	19.87	-
Plant life	20.78	20.62	20.48	20.35	20.24

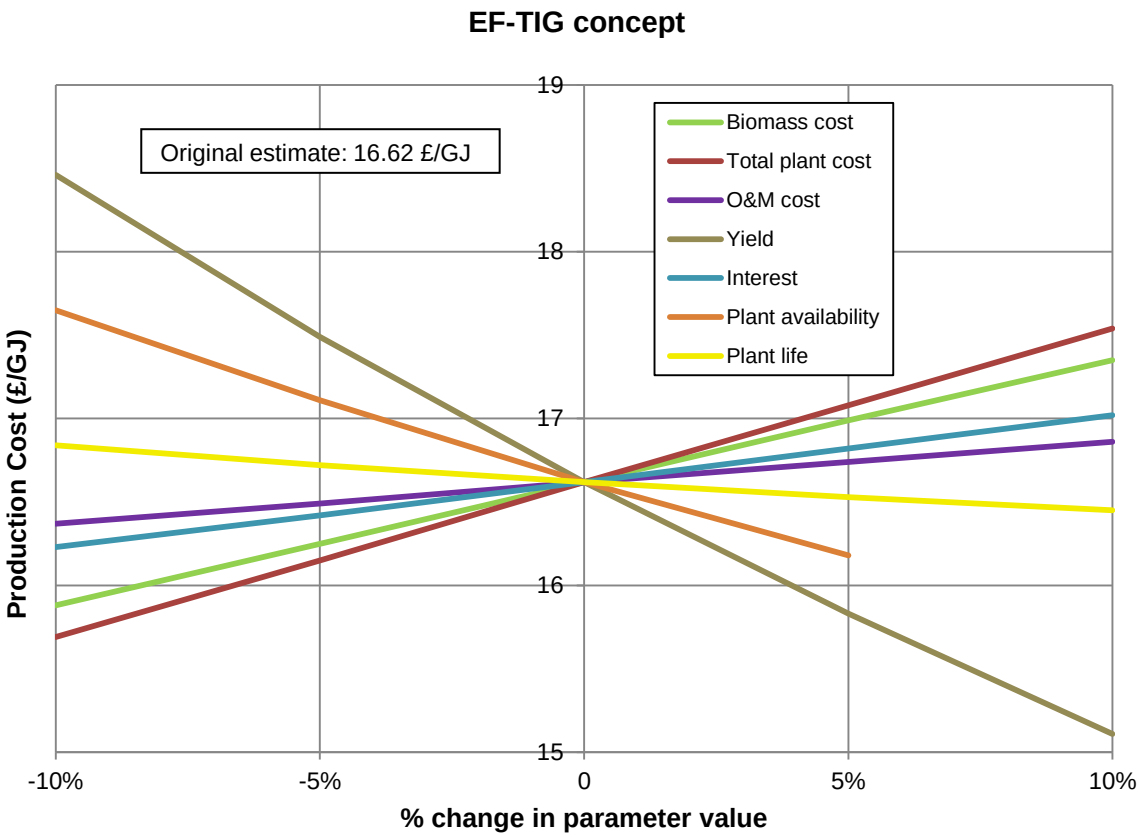


Figure C-3: Sensitivity of biofuels production cost of the EF-TIG concept

Table C-12: Production costs of the EF-TIG concept as a result of parameters' variations

	-10%	-5%	0	5%	10%
Biomass cost	15.88	16.25	16.62	16.99	17.35
Total plant cost	15.69	16.15	16.62	17.08	17.54
O&M cost	16.37	16.49	16.62	16.74	16.86
Yield	18.46	17.49	16.62	15.83	15.11
Interest	16.23	16.42	16.62	16.82	17.02
Plant availability	17.65	17.11	16.62	16.18	
Plant life	16.84	16.72	16.62	16.53	16.45

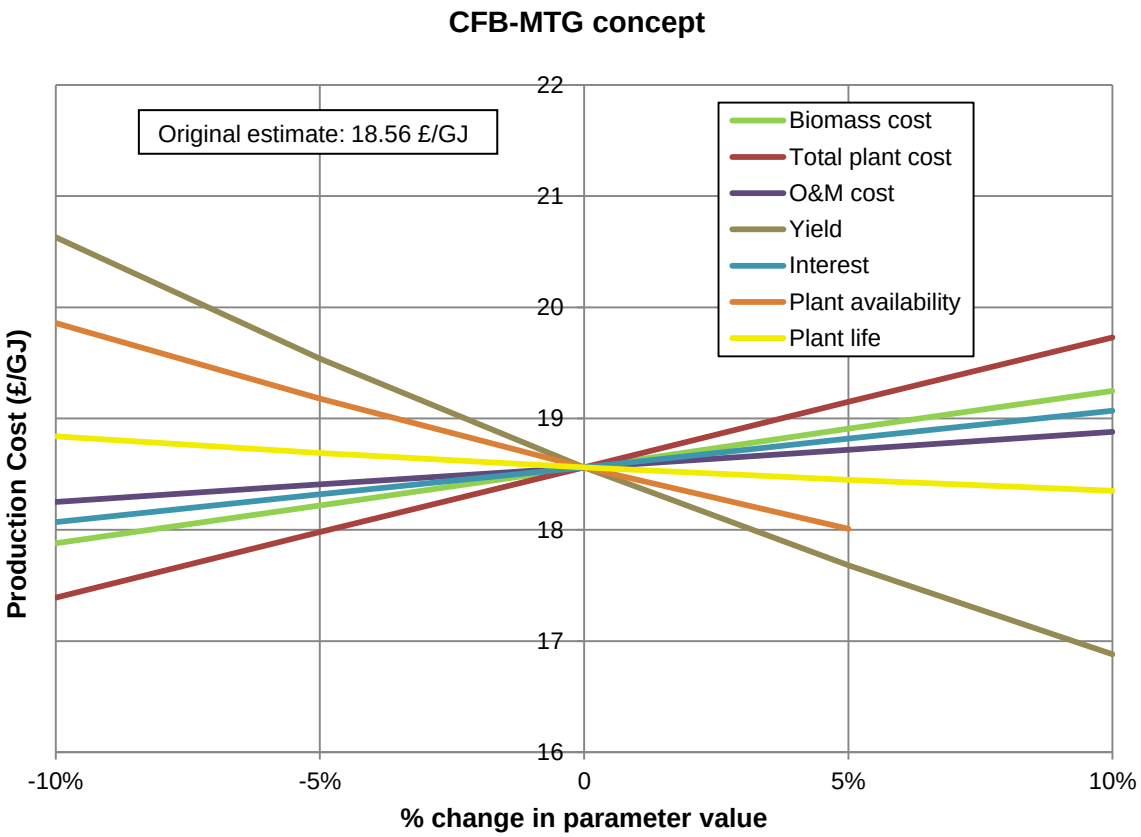


Figure C-4: Sensitivity of biofuels production cost of the CFB-MTG concept

Table C-13: Production costs of the CFB-MTG concept as a result of parameters' variations

	-10%	-5%	0	5%	10%
Biomass cost	17.88	18.22	18.56	18.91	19.25
Total plant cost	17.39	17.98	18.56	19.15	19.73
O&M cost	18.25	18.41	18.56	18.72	18.88
Yield	20.63	19.54	18.56	17.68	16.88
Interest	18.07	18.32	18.56	18.82	19.07
Plant availability	19.86	19.18	18.56	18.01	-
Plant life	18.84	18.69	18.56	18.45	18.35

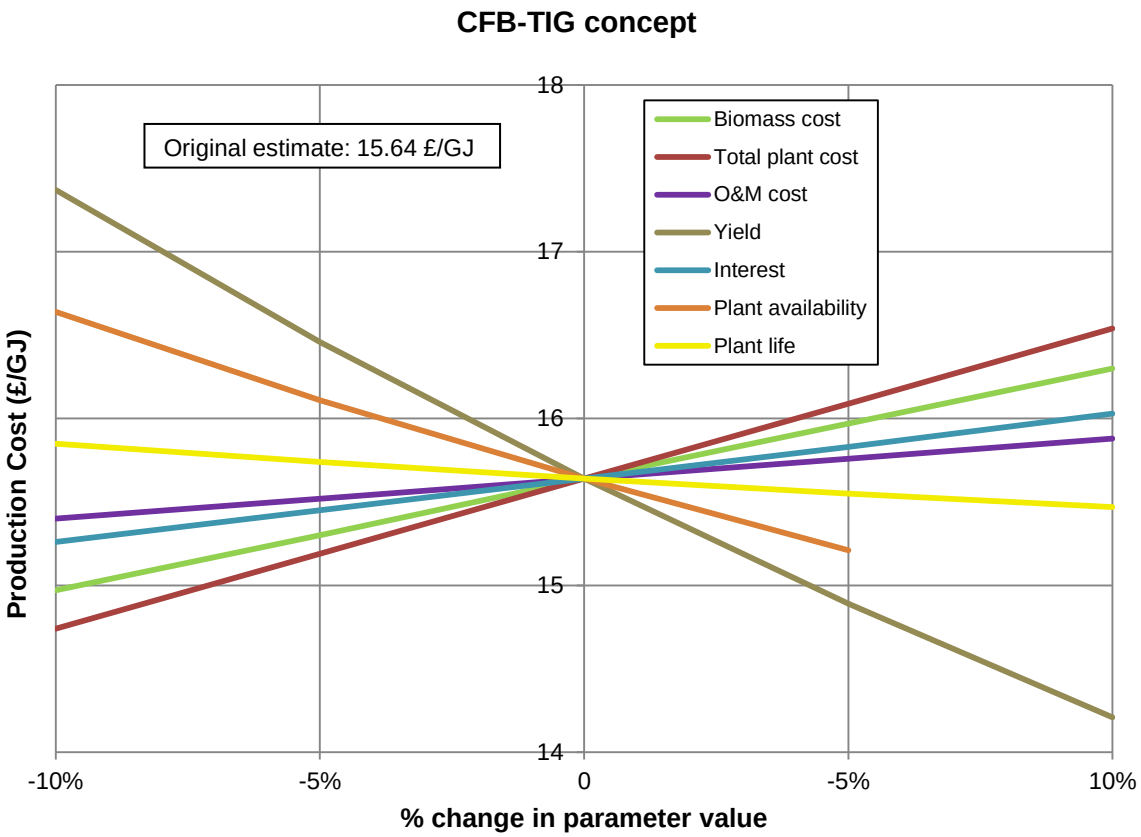


Figure C-5: Sensitivity of biofuels production cost of the CFB-TIG concept

Table C-14: Production costs of the CFB-TIG concept as a result of parameters' variations

	-10%	-5%	0	-5%	10%
Biomass cost	14.97	15.30	15.64	15.97	16.3
Total plant cost	14.74	15.19	15.64	16.09	16.54
O&M cost	15.40	15.52	15.64	15.76	15.88
Yield	17.37	16.46	15.64	14.89	14.21
Interest	15.26	15.45	15.64	15.83	16.03
Plant availability	16.64	16.11	15.64	15.21	-
Plant life	15.85	15.74	15.64	15.55	15.47

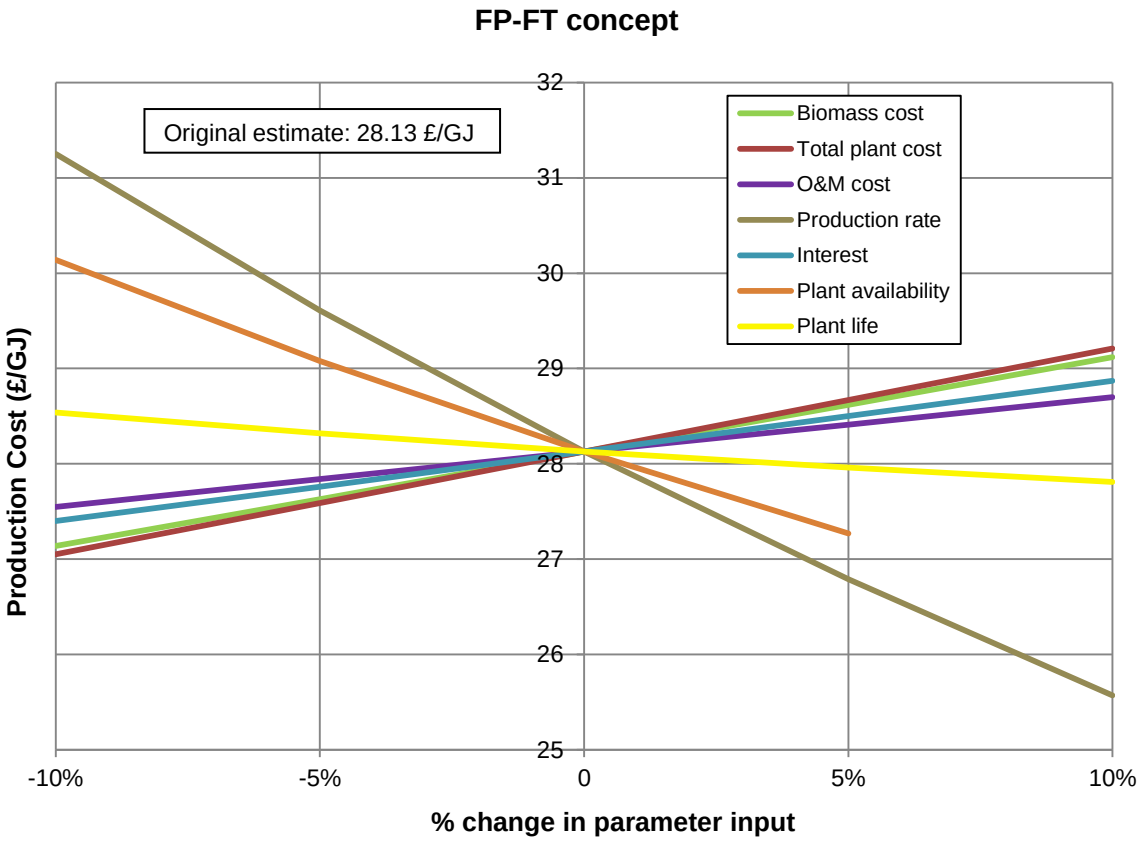


Figure C-6: Sensitivity of biofuels production cost of the FP-FT concept

Table C-15: Production costs of the FP-FT concept as a result of parameters' variations

	-10%	-5%	0	5%	10%
Biomass cost	27.14	27.63	28.13	28.62	29.12
Total plant cost	27.05	27.59	28.13	28.67	29.21
O&M cost	27.55	27.84	28.13	28.41	28.70
Production rate	31.25	29.61	28.13	26.79	25.57
Interest	27.4	27.76	28.13	28.5	28.87
Plant availability	30.14	29.08	28.13	27.27	-
Plant life	28.54	28.32	28.13	27.96	27.81

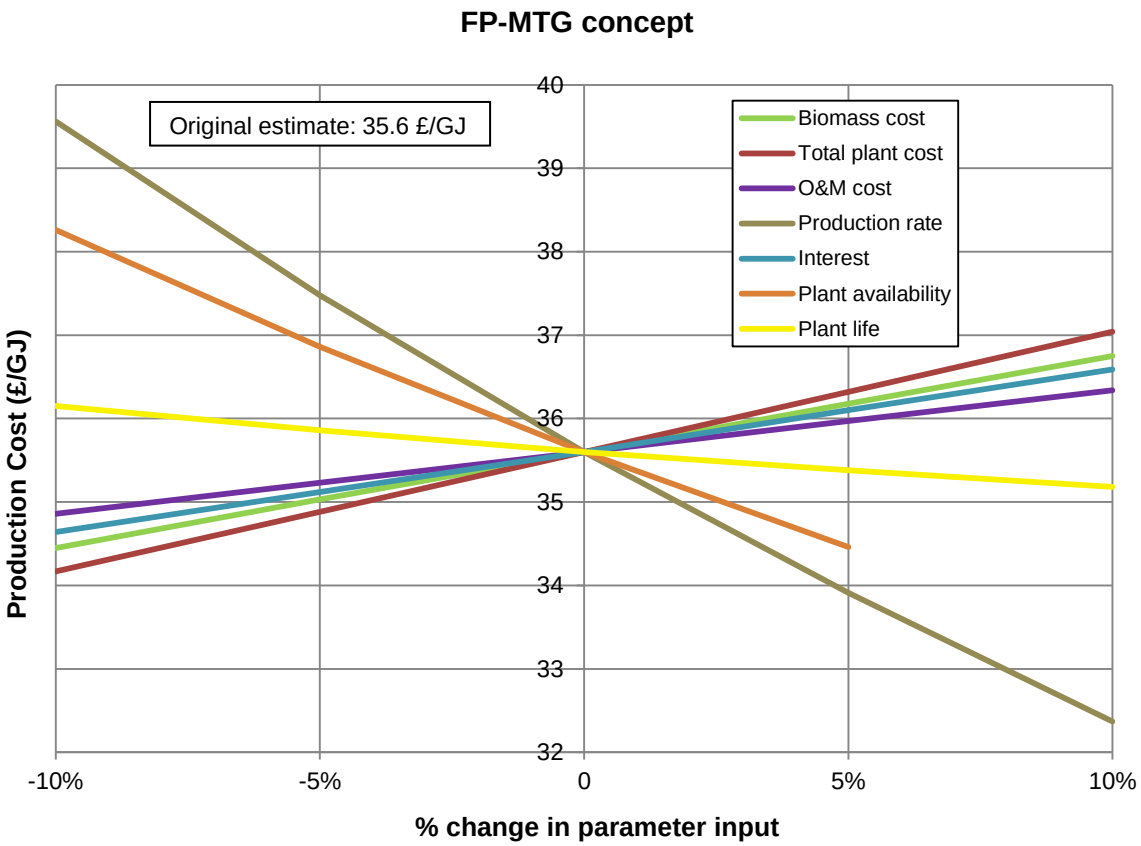


Figure C-7: Sensitivity of biofuels production cost of the FP-MTG concept

Table C-16: Production costs of the FP-MTG concept as a result of parameters' variations

	-10%	-5%	0	5%	10%
Biomass cost	34.45	35.03	35.60	36.18	36.75
Total plant cost	34.17	34.88	35.60	36.32	37.04
O&M cost	34.86	35.23	35.60	35.97	36.34
Production rate	39.56	37.48	35.60	33.91	32.37
Interest	34.64	35.12	35.60	36.10	36.59
Plant availability	38.26	36.86	35.60	34.46	-
Plant life	36.15	35.86	35.60	35.38	35.18

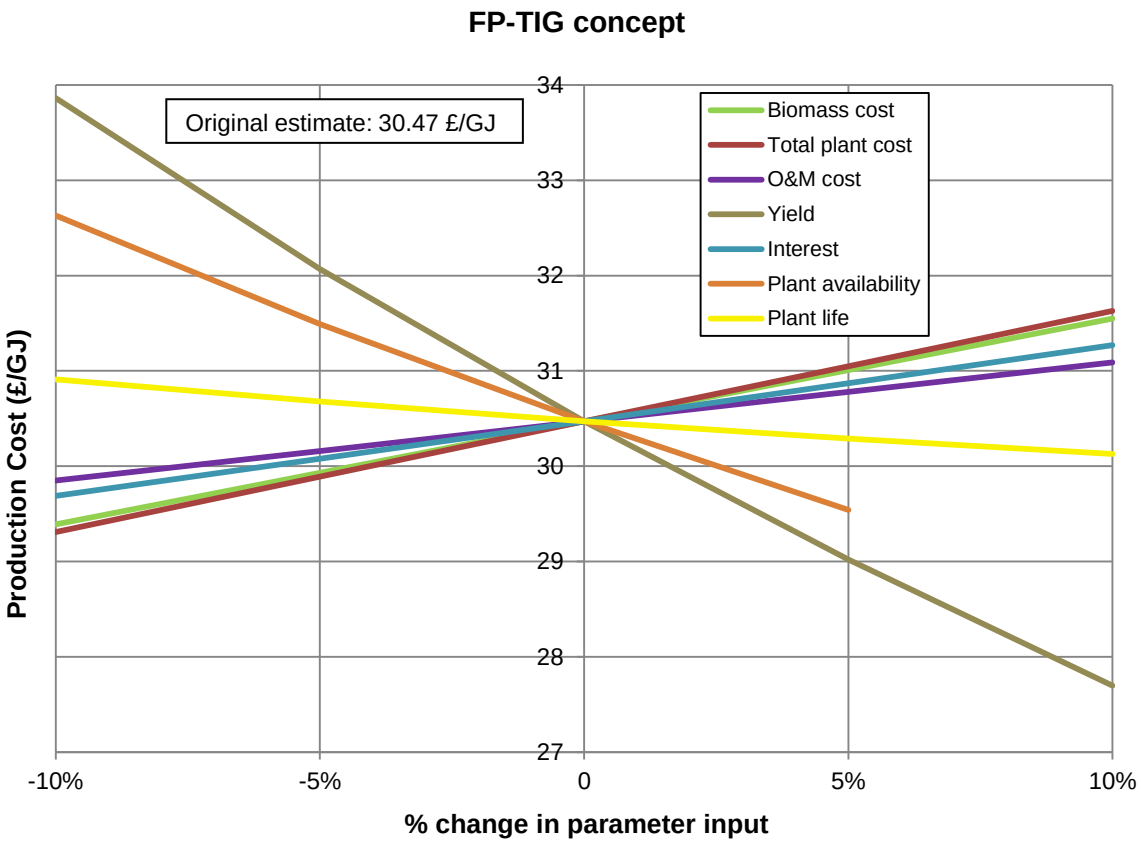


Figure C-8: Sensitivity of biofuels production cost of the FP-TIG concept

Table C-17: Production costs of the FP-TIG concept as a result of parameters' variations

	-10%	-5%	0	5%	10%
Biomass cost	29.39	29.93	30.47	31.01	31.55
Total plant cost	29.31	29.89	30.47	31.05	31.63
O&M cost	29.85	30.16	30.47	30.78	31.09
Yield	33.86	32.07	30.47	29.02	27.7
Interest	29.69	30.08	30.47	30.87	31.27
Plant availability	32.63	31.49	30.47	29.54	-
Plant life	30.91	30.68	30.47	30.29	30.13